THE CLASSICAL MOMENT PROBLEM AS A SELF-ADJOINT FINITE DIFFERENCE OPERATOR

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Abstract. This is a comprehensive exposition of the classical moment problem using methods from the theory of finite difference operators. Among the advantages of this approach is that the Nevanlinna functions appear as elements of a transfer matrix and convergence of Padé approximants appears as the strong resolvent convergence of finite matrix approximations to a Jacobi matrix. As a bonus of this, we obtain new results on the convergence of certain Padé approximants for series of Hamburger.

§1. Introduction

The classical moment problem was central to the development of analysis in the period from 1894 (when Stieltjes wrote his famous memoir [38]) until the 1950's (when Krein completed his series on the subject [15, 16, 17]). The notion of measure (Stieltjes integrals), Padé approximants, orthogonal polynomials, extensions of positive linear functionals (Riesz-Markov theorem), boundary values of analytic functions, and the Herglotz-Nevanlinna-Riesz representation theorem all have their roots firmly in the study of the moment problem.

This expository note attempts to present the main results of the theory with two main ideas in mind. It is known from early on (see below) that a moment problem is associated to a certain semi-infinite Jacobi matrix, A. The first idea is that the basic theorems can be viewed as results on the self-adjoint extensions of A. The second idea is that techniques from the theory of second-order difference and differential equations should be useful in the theory.

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Of course, neither of these ideas is new. Both appear, for example, in Stone's treatment [39], in Dunford-Schwartz [5], and in Akhiezer's brilliant book on the subject [1]. But, normally, (and in [1], in particular), these ideas are presented as applications of the basic theory rather than as the central tenets. By placing them front and center, many parts of the theory become more transparent — in particular, our realization of the Nevanlinna matrix as a transfer matrix makes its properties (as an entire function of order 1 and minimal type) evident (see Theorem 4.8 below).

Two basic moment problems will concern us here:

Hamburger Moment Problem. Given a sequence $\gamma_0, \gamma_1, \gamma_2, \dots$ of reals, when is there a measure, $d\rho$, on $(-\infty, \infty)$ so that

$$\gamma_n = \int_{-\infty}^{\infty} x^n \, d\rho(x) \tag{1.1}$$

and if such a ρ exists, is it unique? We let $\mathcal{M}_H(\gamma)$ denote the set of solutions of (1.1).

Stieltjes Moment Problem. Given a sequence $\gamma_0, \gamma_1, \gamma_2, \dots$ of reals, when is there a measure, $d\rho$ on $[0, \infty)$ so that

$$\gamma_n = \int_0^{\infty} x^n \, d\rho(x) \tag{1.2}$$

and if such a ρ exists, is it unique? We let $\mathcal{M}_S(\gamma)$ denote the set of solutions of (1.2).

We will not attempt a comprehensive historical attribution of classical results; see Akhiezer [1] and Shohat-Tamarkin [35] for that.

We will always normalize the γ's so that $\gamma_0 = 1$. By replacing γ_n by γ_n/γ_0, we can reduce general γ's to this normalized case. We will also demand that $d\rho$ have infinite support, that is, that ρ not be a pure point measure supported on a finite set. This eliminates certain degenerate cases.

One immediately defines two sesquilinear forms, H_N and S_N, on $\mathbb{C}^N$ for each N by

$$H_N(\alpha, \beta) = \sum_{\substack{n=0,1,\dots,N-1 \\ m=0,1,\dots,N-1}} \bar{\alpha}_n \beta_m \gamma_{n+m} \tag{1.3}$$

$$S_N(\alpha, \beta) = \sum_{\substack{n=0,1,\dots,N-1 \\ m=0,1,\dots,N-1}} \bar{\alpha}_n \beta_m \gamma_{n+m+1} \tag{1.4}$$

and corresponding matrices $\mathcal{H}_N$ and $\mathcal{S}_N$ so that $H_N(\alpha, \beta) = \langle \alpha, \mathcal{H}_N \beta \rangle$ and $S_N(\alpha, \beta) = \langle \alpha, \mathcal{S}_N \beta \rangle$ in the usual Euclidean inner product. Our inner products are linear in the second factor and anti-linear in the first.

A standard piece of linear algebra says:

Lemma 1.1. *An $N \times N$ Hermitean matrix A is strictly positive definite if and only if each submatrix $A^{[1,J]} = (a_{ij})_{1 \le i,j \le J}$ has $\det(A^{[1,J]}) > 0$ for $J = 1, 2, \dots, N$.*

Proof. If A is strictly positive definite, so is each $A^{[1,J]}$, so their eigenvalues are all strictly positive and so their determinants are all strictly positive.

For the converse, suppose that $A^{[1,N-1]}$ is positive definite. By the min-max principle, the $(N-1)$ eigenvalues of $A^{[1,N-1]}$ interlace the N eigenvalues of $A^{[1,N]} \equiv A$. If all the eigenvalues of $A^{[1,N-1]}$ are positive, so are the $N-1$ largest eigenvalues of A. If the N^{th} eigenvalue were non-positive, $\det(A) \le 0$. Thus, $A^{[1,N-1]}$ strictly positive definite and $\det(A^{[N,N]}) > 0$ imply $A^{[1,N]}$ is strictly positive definite. An obvious induction completes the proof. □

This immediately implies

Proposition 1.2. *$\{H_N\}_{N=1}^{\infty}$ are strictly positive definite forms if and only if $\det(\mathcal{H}_N) > 0$ for $N = 1, 2, \dots$. Similarly, $\{S_N\}_{N=1}^{\infty}$ are strictly positive definite forms if and only if $\det(\mathcal{S}_N) > 0$ for $N = 1, 2, \dots$.*

Suppose that the γ_n obey (1.1). Then by an elementary calculation,

$$\int \left| \sum_{n=0}^{N-1} \alpha_n x^n \right|^2 d\rho(x) = H_N(\alpha, \alpha) \tag{1.5}$$

$$\int x \left| \sum_{n=0}^{N-1} \alpha_n x^n \right|^2 d\rho(x) = S_N(\alpha, \alpha). \tag{1.6}$$

Taking into account that if $\int |P(x)|^2 \, d\rho(x) = 0$, ρ must be supported on the zeros of P, we have:

Proposition 1.3. *A necessary condition that (1.1) holds for some measure $d\rho$ on $(-\infty, \infty)$ with infinite support is that each sesquilinear form H_N is strictly positive definite. A necessary condition that there be a $d\rho$ supported on $[0, \infty)$ is that each H_N and each S_N be strictly positive definite.*

Suppose now that each H_N is strictly positive definite. Let $\mathbb{C}[X]$ be the family of complex polynomials. Given $P(X) = \sum_{n=0}^{N-1} \alpha_n X^n$, $Q(X) = \sum_{n=0}^{N-1} \beta_n X^n$ (we suppose the upper limits in the sums are equal by using some zero α's or β's if need be), define

$$\langle P, Q \rangle = H_N(\alpha, \beta). \tag{1.7}$$

This defines a positive definite inner product on $\mathbb{C}[X]$, and, in the usual way, we can complete $\mathbb{C}[X]$ to a Hilbert space $\mathcal{H}^{(\gamma)}$ in which $\mathbb{C}[X]$ is dense. $\mathbb{C}[X]$ can be thought of as abstract polynomials or as infinite sequences $(\alpha_0, \alpha_1, \dots, \alpha_{N-1}, 0, \dots)$ which are eventually 0 via $\alpha \sim \sum_{j=0}^{N-1} \alpha_j X^j$.

We will start using some basic facts about symmetric and self-adjoint operators on a Hilbert space — specifically, the spectral theorem and the von Neumann theory of

self-adjoint extensions. For an exposition of these ideas, see Chapters VII, VIII, and X of Reed-Simon, volumes I and II [33, 34] and see our brief sketch at the start of Section 2.

Define a densely defined operator A on $\mathcal{H}^{(\gamma)}$ with domain $D(A) = \mathbb{C}[X]$ by

$$A[P(X)] = [XP(X)]. \tag{1.8}$$

In the sequence way of looking at things, A is the right shift, that is, $A(\alpha_0, \alpha_1, \dots, \alpha_N, 0, \dots) = (0, \alpha_0, \alpha_1, \dots, \alpha_N, 0, \dots)$. This means that

$$\langle P, A[Q]\rangle = S_N(\alpha, \beta) \tag{1.9}$$

and, in particular,

$$\langle 1, A^n 1\rangle = \gamma_n. \tag{1.10}$$

Since $\mathcal{H}_N$ and $\mathcal{S}_N$ are real-symmetric matrices, A is a symmetric operator, that is, $\langle A[P], Q\rangle = \langle P, A[Q]\rangle$. Moreover, if we define a complex conjugation C on $\mathbb{C}[X]$ by $C(\sum_{n=0}^{N-1} \alpha_n X^n) = \sum_{n=0}^{N-1} \bar{\alpha}_n X^n$, then $CA = AC$. It follows by a theorem of von Neumann (see Corollary 2.4 in Section 2) that A has self-adjoint extensions.

If each S_N is positive definite, then $\langle P, A[P]\rangle \geq 0$ for all P, and it follows that A has a non-negative self-adjoint extension A_F, the Friedrichs extension (discussed further in Section 3). We thus see:

Proposition 1.4. *If all H_N are positive definite, then A has self-adjoint extensions. If all S_N are positive definite, then A has non-negative self-adjoint extensions.*

Let $\tilde{A}$ be a self-adjoint extension of A. By the spectral theorem, there is a spectral measure $d\tilde{\mu}$ for $\tilde{A}$ with vector $[1] \in \mathcal{H}^{(\gamma)}$, that is, so that for any bounded function of $\tilde{A}$,

$$\langle 1, f(\tilde{A})1\rangle = \int f(x)\, d\tilde{\mu}(x). \tag{1.11}$$

Since $1 \in D(A^N) \subset D(\tilde{A}^N)$, (1.11) extends to polynomially bounded functions and we have by (1.10) that,

$$\gamma_N = \int x^N \, d\tilde{\mu}(x).$$

We see therefore that a self-adjoint extension of A yields a solution of the Hamburger moment problem. Moreover, a non-negative self-adjoint extension has $\operatorname{supp}(d\tilde{\mu}) \subset [0, \infty)$ and so yields a solution of the Stieltjes moment problem. Combining this with Propositions 1.2, 1.3, and 1.4, we have the first major result in the theory of moments.

Theorem 1 (Existence). *A necessary and sufficient condition for there to exist a measure $d\rho$ with infinite support obeying* (1.1) *is that* $\det(\mathcal{H}_N) > 0$ *for* $N = 1, 2, \dots$. *A necessary and sufficient condition that also $d\rho$ be supported on* $[0, \infty)$ *is that both* $\det(\mathcal{H}_N) > 0$ *and* $\det(\mathcal{S}_N) > 0$ *for* $N = 1, 2, \dots$.

Historically, existence was a major theme because the now standard tools on existence of measures were invented in the context of moment problems. We have settled it quickly,

and the bulk of this paper is devoted to uniqueness, especially the study of cases of non-uniqueness. Non-uniqueness only occurs in somewhat pathological situations, but the theory is so elegant and beautiful that it has captivated analysts for a century.

Henceforth, we will call a set of moments $\{\gamma_n\}_{n=0}^\infty$ with $\det(\mathcal{H}_N) > 0$ for all N a set of *Hamburger moments*. If both $\det(\mathcal{H}_N) > 0$ and $\det(\mathcal{S}_N) > 0$ for all N, we call them a set of *Stieltjes moments*.

We will call a solution of the moment problem which comes from a self-adjoint extension of A a *von Neumann solution*. The name is in honor of the use below of the von Neumann theory of self-adjoint extensions of densely-defined symmetric operators. This name, like our use of Friedrichs solution and Krein solution later, is not standard, but it is natural from the point of view of self-adjoint operators. As far as I know, neither von Neumann nor Friedrichs worked on the moment problem per se. While Krein did, his work on the moment problem was not in the context of the Krein extension we use to construct what we will call the Krein solution. What we call von Neumann solutions, Akhiezer calls N-extremal and Shohat-Tamarkin call extremal. This last name is unfortunate since we will see there exist many solutions which are extreme points in the sense of convex set theory, but which are not von Neumann solutions (and so, not extremal in the Shohat-Tamarkin sense).

Given the connection with self-adjoint extensions, the following result is reasonable (and true!):

Theorem 2 (Uniqueness). *A necessary and sufficient condition that the measure $d\rho$ in* (1.1) *be unique is that the operator A of* (1.8) *is essentially self-adjoint* (*i.e., has a unique self-adjoint extension*). *A necessary and sufficient condition that there be a unique measure $d\rho$ in* (1.1) *supported in* $[0,\infty)$ *is that A have a unique non-negative self-adjoint extension.*

This result is surprisingly subtle. First of all, it is not obvious (but true, as we will see) that distinct self-adjoint extensions have distinct spectral measures $d\tilde{\mu}$, so there is something to be proven before multiple self-adjoint extensions imply multiple solutions of the moment problem. The other direction is even less clear cut, for not only is it not obvious, it is false that every solution of the moment problem is a von Neumann solution (Reed-Simon [34] has an incorrect proof of uniqueness that implicitly assumes every solution comes from a self-adjoint extension). As we will see, once there are multiple solutions, there are many, many more solutions than those that come from self-adjoint extensions in the von Neumann sense of looking for extensions in $\overline{D(A)}$. But, as we will see in Section 6, there is a sense in which solutions are associated to self-adjoint operators in a larger space.

We also note we will see cases where the Stieltjes problem has a unique solution but the associated Hamburger problem does not.

The Hamburger part of Theorem 2 will be proven in Section 2 (Theorems 2.10 and 2.12); the Stieltjes part will be proven in Sections 2 and 3 (Theorems 2.12 and 3.2). If there is a unique solution to (1.1), the moment problem is called *determinate*; if there are multiple solutions, it is called *indeterminate*. It is ironic that the English language

literature uses these awkward terms, rather than determined and undetermined. Stieltjes was Dutch, but his fundamental paper was in French, and the names have stuck. Much of the interesting theory involves analyzing the indeterminate case, so we may as well give some examples that illuminate non-uniqueness.

Example 1.1. Let f be a non-zero C^∞ function on $\mathbb{R}$ supported on $[0,1]$. Let $g(x) = \hat{f}(x)$, with $\hat{f}$ the Fourier transform of f. Then

$$\int_{-\infty}^{\infty} x^n g(x)\, dx = \sqrt{2\pi}\,(-i)^n \frac{d^n f}{dx^n}(0) = 0.$$

Let $d\rho_1(x) = (\operatorname{Re} g)_+(x)\, dx$, the positive part of $\operatorname{Re} g$, and let $d\rho_2 = (\operatorname{Re} g)_-(x)\, dx$. By the above,

$$\int_{-\infty}^{\infty} x^n d\rho_1(x) = \int_{-\infty}^{\infty} x^n\, d\rho_2(x)$$

for all n. Since $d\rho_1$ and $d\rho_2$ have disjoint essential supports, they are unequal and we have non-unique solutions of the moment problem. (We will see eventually that neither is a von Neumann solution.) The moments from ρ_1, ρ_2 may not be normalized. But we clearly have non-uniqueness after normalization.

This non-uniqueness is associated to non-analyticity in a Fourier transform and suggests that if one can guarantee analyticity, one has uniqueness. Indeed,

Proposition 1.5. *Suppose that $\{\gamma_n\}_{n=0}^\infty$ is a set of Hamburger moments and that for some $C, R > 0$,*

$$|\gamma_n| \le CR^n n! \tag{1.12a}$$

Then the Hamburger moment problem is determinate.

If $\{\gamma_n\}_{n=0}^\infty$ is a set of Stieltjes moments and

$$|\gamma_n| \le CR^n (2n)! \tag{1.12b}$$

then the Stieltjes moment problem is determinate.

Proof. Let $d\rho$ obey (1.1). Then $x^{2n} \in L^1(\mathbb{R}, d\rho)$, and by the monotone convergence theorem,

$$\begin{aligned}\int_{-\infty}^{\infty} \cosh\left(\frac{x}{2R}\right) d\rho(x) &= \lim_{N\to\infty} \int_{-\infty}^{\infty} \sum_{n=0}^{N} \left(\frac{x}{2R}\right)^{2n} \frac{1}{(2n)!}\, d\rho(x) \\ &\le C \lim_{N\to\infty} \sum_{n=0}^{N} \left(\frac{1}{2}\right)^{2n} = \frac{4}{3} C < \infty.\end{aligned}$$

Thus, $e^{\alpha x} \in L^1(\mathbb{R}, d\rho(x))$ for $|\alpha| < \frac{1}{2R}$. It follows that $F_\rho(z) \equiv \int e^{izx} d\rho(x)$ has an analytic continuation to $\{z \mid |\operatorname{Im} z| < \frac{1}{2R}\}$. If μ is a second solution of (1.1), $F_\mu(z)$ is

also analytic there. But $-i^n \frac{d^n F_\rho}{dz}(0) = \gamma_n$, so the Taylor series of F_ρ and F_μ at $z = 0$ agree, so $F_\rho = F_\mu$ in the entire strip by analyticity.

This implies that $\mu = \rho$ by a variety of means. For example, in the topology of bounded uniformly local convergence, (i.e., $f_n \to f$ means $\sup \|f_n\|_\infty < 0$ and $f_n(x) \to f(x)$ uniformly for x in any $[-\kappa, \kappa]$), linear combinations of the $\{e^{iyx} \mid y \in \mathbb{R}\}$ are dense in all bounded continuous functions. Or alternatively, $G_\mu(z) = \int \frac{d\mu(x)}{x-z} = i \int_{-\infty}^{0} e^{-iyz} F_\mu(y)\, dy$ for $\operatorname{Im} z > 0$, and μ can be recovered as a boundary value of G_μ.

The $(2n)!$ Stieltjes result follows from the $n!$ result and Proposition 1.6 below. $\square$

We will generalize Proposition 1.5 later (see Corollary 4.5).

Proposition 1.6. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Stieltjes moments. Let*

$$\begin{aligned} \Gamma_{2m} &= \gamma_m, \qquad && m = 0, 1, \dots \\ \Gamma_{2m+1} &= 0, && m = 0, 1, \dots. \end{aligned}$$

If $\{\Gamma_j\}_{j=0}^\infty$ is a determinate Hamburger problem, then $\{\gamma_n\}_{n=0}^\infty$ is a determinate Stieljes problem.

Proof. Let $d\rho$ solve the Stieltjes problem. Let

$$d\mu(x) = \tfrac{1}{2}[\chi_{[0,\infty)}(x)\, d\rho(x^2) + \chi_{(-\infty,0]}(x)\, d\rho(x^2)].$$

Then the moments of μ are Γ. Thus uniqueness for the Γ problem on $(-\infty, \infty)$ implies uniqueness for the γ problem on $[0, \infty)$. $\square$

Remark. We will see later (Theorem 2.13) that the converse of the last assertion in Proposition 1.6 is true. This is a more subtle result.

Example 1.2. This example is due to Stieltjes [38]. It is interesting for us here because it is totally explicit and because it provides an example of non-uniqueness for the Stieltjes moment problem. Note first that

$$\int_0^\infty u^k u^{-\ln u} \sin(2\pi \ln u)\, du = 0.$$

This follows by the change of variables $v = -\frac{k+1}{2} + \ln u$, the periodicity of $\sin(\,\cdot\,)$, and the fact that sin is an odd function. Thus for any $\theta \in [-1, 1]$,

$$\frac{1}{\sqrt{\pi}} \int_0^\infty u^k u^{-\ln u} [1 + \theta \sin(2\pi \ln u)]\, du = e^{\frac{1}{4}(k+1)^2}$$

(by the same change of variables) so $\gamma_k = e^{\frac{1}{4}(k+1)^2}$ is an indeterminate set of Stieltjes moments. Notice for $\theta \in (-1, 1)$, if $d\rho_\theta(u)$ is the measure with these moments, then $\sin(2\pi \ln(u))/1+\theta \sin(2\pi \ln(u))$ is in $L^2(d\rho_\theta)$ and orthogonal to all polynomials, so $d\rho_\theta(u)$ is a measure with all moments finite but where the polynomials are not L^2 dense. As

we shall see, this is typical of solutions of indeterminate moment problems which are not von Neumann solutions.

Looking at the rapid growth of the moments in Example 1.2, you might hope that just as a condition of not too great growth (like Proposition 1.5) implies determinacy, there might be a condition of rapid growth that implies indeterminacy. But that is false! There are moments of essentially arbitrary rates of growth which lead to determinate problems (see the remark after Corollary 4.21 and Theorem 6.2).

Example 1.3. There is a criterion of Krein [18] for indeterminacy that again shows the indeterminacy of Example 1.2, also of the example of the moments of $\exp(-|x|^\alpha)\,dx$ (on $(-\infty,\infty)$) with $\alpha<1$ and also an example of Hamburger [8], the moments of

$$\chi_{[0,\infty)}(x)\exp\left(-\frac{\pi\sqrt{x}}{\ln^2 x+\pi^2}\right)dx.$$

Proposition 1.7 (Krein [18]). *Suppose that $d\rho(x)=F(x)\,dx$ where $0\le F(x)\le 1$ and either*

(i) $\operatorname{supp}(F)=(-\infty,\infty)$ *and*

$$\int_{-\infty}^{\infty} -\frac{\ln(F(x))}{1+x^2}\,dx<\infty \tag{1.13a}$$

or

(ii) $\operatorname{supp}(F)=[0,\infty)$ *and*

$$\int_0^\infty -\frac{\ln(F(x))}{(1+x)}\,\frac{dx}{\sqrt{x}}<\infty. \tag{1.13b}$$

Suppose also that for all n:

$$\int_{-\infty}^{\infty}|x|^n F(x)\,dx<\infty. \tag{1.13c}$$

Then the moment problem (*Hamburger in case* (i), *Stieltjes in case* (ii)) *with moments*

$$\gamma_n=\frac{\int x^n F(x)\,dx}{\int F(x)\,dx}$$

is indeterminate.

Remarks. 1. Hamburger's example is close to borderline for (1.13b) to hold.

2. Since $\int_{-\infty}^\infty x^{2n}\exp(-|x|^\alpha)\,dx=2\alpha^{-1}\Gamma(\frac{2n+1}{\alpha})\sim(\frac{2n}{\alpha})!$ and (1.13a) holds for $F(x)=\exp(-|x|^\alpha)$ if $\alpha<1$, we see that there are examples of Hamburger indeterminate moment problems with growth just slightly faster than the $n!$ growth, which would imply by Proposition 1.5 that the problem is determinate. Similarly, since $\int_0^\infty x^n\exp(-|x|^\alpha)\,dx=$

$\alpha^{-1}\Gamma(\frac{n+1}{\alpha}) \sim (\frac{n}{\alpha})!$ and (1.13b) holds for $F(x) = \exp(-|x|^\alpha)$ if $\alpha < \frac{1}{2}$, we see there are examples of Stieltjes indeterminate problems with growth just slightly faster than the $(2n)!$ of Proposition 1.5.

3. Since $F(x) = \frac{1}{2}e^{-|x|}$ has moments $\gamma_{2n} = (2n)!$ covered by Proposition 1.5, it is a determinate problem. The integral in (1.13a) is only barely divergent in this case. Similarly, $F(x) = \chi_{[0,\infty)}(x)e^{-\sqrt{x}}$ is a Stieltjes determinate moment problem by Proposition 1.5 and the integral in (1.13b) is barely divergent. This says that Krein's conditions are close to optimal.

4. Krein actually proved a stronger result by essentially the same method. F need not be bounded (by a limiting argument from the bounded case) and the measure defining γ_n can have an arbitrary singular part. Moreover, Krein proves (1.13a) is necessary and sufficient for $\{e^{i\alpha x}\}_{0\le\alpha<\infty}$ to not be dense in $L^2(\mathbb{R}, F(x)\,dx)$.

5. Krein's construction, as we shall see, involves finding a bounded analytic function G in $\mathbb{C}_+ \equiv \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}$ so that $|G(x+i0)| \le F(x)$. From this point of view, the fact that $F(x)$ cannot decay faster than $e^{-|x|}$ is connected to the Phragmén-Lindelöf principle.

6. The analog of Krein's result for the circle instead of the half plane is due to Szego.

Proof. Suppose we can find G with $\operatorname{Re} G \not\equiv 0$ with $|G(x)| \le F(x)$ so that

$$\int x^n G(x)\,dx = 0.$$

Then both $\frac{F(x)\,dx}{\int F(x)\,dx}$ and $\frac{[F(x)+\operatorname{Re} G(x)]\,dx}{\int F(x)\,dx}$ solve the γ_n moment problem, showing indeterminacy.

In case (i), define for $z \in \mathbb{C}_+$ (see (1.19) and the definition of Herglotz function below):

$$Q(z) = \frac{1}{\pi}\int\left(\frac{1}{x-z} - \frac{x}{1+x^2}\right)[-\ln(F(x))]\,dx,$$

which is a convergent integral by (1.13a). Then, $\operatorname{Im} Q(z) \ge 0$ and by the theory of boundary values at such analytic functions [13], $\lim_{\varepsilon\downarrow 0} Q(x+i\varepsilon) \equiv Q(x+i0)$ exists for a.e. $x \in \mathbb{R}$ and $\operatorname{Im} Q(x+i0) = -\ln F(x)$.

Let $G(z) = \exp(iQ(z))$ for $z \in \mathbb{C}_+$ and $G(x) = \exp(iQ(x+i0))$. Then the properties of Q imply $|G(z)| \le 1$, $\lim_{\varepsilon\downarrow 0} G(x+i0) = G(x)$ for a.e. x in $\mathbb{R}$, and $|G(x)| = F(x)$. A standard contour integral argument then shows that for any $\varepsilon > 0$ and $n > 0$,

$$\int x^n(1-i\varepsilon x)^{-n-2}G(x)\,dx = 0.$$

Since (1.13c) holds and $|G(x)| \le F(x)$, we can take $\varepsilon \downarrow 0$ and obtain $\int x^n G(x)\,dx = 0$.

In case (ii), define

$$Q(z) = \frac{2z}{\pi}\int_0^\infty -\frac{\ln F(x^2)}{x^2-z^2}\,dx.$$

Again, the integral converges by (1.13b) and $\operatorname{Im} Q(z) > 0$. Moreover, $Q(-\bar{z}) = -\overline{Q(z)}$. We have for a.e. $x \in \mathbb{R}$, $\operatorname{Im} Q(x+i0) = -\ln F(x^2)$. Thus, if $H(z) = \exp(iQ(z))$ for $z \in \mathbb{C}_+$ and $H(x) = \exp(iQ(x+i0))$ for $x \in \mathbb{R}$ and $G(x) = \operatorname{Im} H(\sqrt{x})$ for $x \in [0,\infty)$, then, as above,

$$\int_{-\infty}^{\infty} x^{2n+1} H(x)\, dx = 0,$$

so since $H(-x) = \overline{H(x)}$, $\int_0^\infty x^{2n+1} G(x^2)\, dx = 0$ or $\int_0^\infty y^n G(y)\, dy = 0$. Since $|H(x)| = F(x^2)$, we have that $|G(x)| \leq F(x)$. $\square$

Additional examples of indeterminate moment problems (specified by their orthogonal polynomials) can be found in [9, 10].

One point to note for now is that in all these examples, we have non-uniqueness with measures $d\rho$ of the form $d\rho(x) = G(x)\, dx$ (i.e., absolutely continuous). This will have significance after we discuss Theorem 5 below.

To discuss the theory further, we must look more closely at the operator A given by (1.8). Consider the set $\{1, X, X^2, \dots\}$ in $\mathcal{H}^{(\gamma)}$. By the strict positivity of H_N, these elements in $\mathcal{H}^{(\gamma)}$ are linearly independent and they span $\mathcal{H}^{(\gamma)}$ by construction. Thus by a Gram-Schmidt procedure, we can obtain an orthogonal basis, $\{P_n(X)\}_{n=0}^\infty$, for $\mathcal{H}^{(\gamma)}$. By construction,

$$P_n(X) = c_{nn} X^n + \text{ lower order}, \qquad \text{with } c_{nn} > 0 \tag{1.14a}$$

$$\langle P_n, P_m \rangle = 0, \qquad m = 0, 1, 2, \dots, n-1 \tag{1.14b}$$

$$\langle P_n, P_n \rangle = 1. \tag{1.14c}$$

These are, of course, the well-known orthogonal polynomials for $d\rho$ determined by the moments $\{\gamma_n\}_{n=0}^\infty$. Note that often the normalization condition (1.14c) is replaced by $c_{nn} \equiv 1$, yielding a distinct set of "orthogonal" polynomials. There are explicit formulae for the $P_n(X)$ in terms of determinants and the γ's. We discuss them in Appendix A.

By construction, $\{P_j\}_{j=0}^n$ is an orthonormal basis for the polynomials of degree n. The realization of elements of $\mathcal{H}^{(\gamma)}$ as $\sum_{n=0}^\infty \lambda_n P_n(X)$ with $\sum_{n=0}^\infty |\lambda_n|^2 < \infty$ gives a different realization of $\mathcal{H}^{(\gamma)}$ as a set of sequences $\lambda = (\lambda_0, \dots)$ with the usual $\ell^2(\{0,1,2,\dots\})$ inner product. $\mathbb{C}[X]$ corresponds to these λ's with $\lambda_n = 0$ for n sufficiently large. But we need to bear in mind this change of realization as sequences.

Note that $\operatorname{span}[1, \dots, X^n] = \operatorname{span}[P_0, \dots, P_n(X)]$. In particular, $XP_n(X)$ has an expansion in $P_0, P_1, \dots, P_{n+1}$. But $\langle XP_n, P_j \rangle = \langle P_n, XP_j \rangle = 0$ if $j < n-1$ since then XP_j is of degree at most $n-1$, and (1.14b) holds. Thus for suitable sequences, $\{a_n\}_{n=0}^\infty$, $\{b_n\}_{n=0}^\infty$, and $\{c_n\}_{n=0}^\infty$ (with $P_{-1}(X) \equiv 0$),

$$XP_n(X) = c_n P_{n+1}(X) + b_n P_n(X) + a_{n-1} P_{n-1}(X) \tag{1.15}$$

for $n = 0, 1, 2, \dots$. Notice that by (1.14a), $c_n > 0$ and

$$c_n = \langle P_{n+1}, XP_n \rangle = \langle P_n, XP_{n+1} \rangle = a_n.$$

(1.15) thus becomes

$$XP_n(X) = a_n P_{n+1}(X) + b_n P_n(X) + a_{n-1} P_{n-1}(X). \tag{1.15$'$}$$

Since $\{P_n(X)\}$ are an orthonormal basis for $\mathcal{H}^{(\gamma)}$, this says that in this basis, A is given by a tridiagonal matrix, and $D(A)$ is the set of sequences of finite support.

Thus, given a set $\{\gamma_n\}_{n=0}^{\infty}$ of Hamburger moments, we can find $b_0, b_1, \dots$ real and $a_0, a_1, \dots$ positive so that the moment problem is associated to self-adjoint extensions of the Jacobi matrix,

$$A = \begin{pmatrix} b_0 & a_0 & 0 & 0 & \dots \\ a_0 & b_1 & a_1 & 0 & \dots \\ 0 & a_1 & b_2 & a_2 & \dots \\ 0 & 0 & a_2 & b_3 & \dots \\ \dots & \dots & \dots & \dots & \dots \end{pmatrix}. \tag{1.16}$$

There are explicit formulae for the b_n's and a_n's in terms of the determinants of the γ_n's. We will discuss them in Appendix A.

Conversely, given a matrix A of the form (1.16), we can find a set of moments for which it is the associated Jacobi matrix. Indeed, if δ_0 is the vector $(1, 0, \dots, 0, \dots)$ in ℓ_2, then

$$\gamma_n = (\delta_0, A^n \delta_0).$$

Thus the theory of Hamburger moments is the theory of semi-infinite Jacobi matrices.

So far we have considered the $P_n(X)$ as abstract polynomials, one for each n. It is useful to turn this around. First, replace the abstract X by an explicit complex number. For each such z, consider the semi-infinite sequence $\pi(z) = (P_0(z), P_1(z), P_2(z), \dots)$. (1.15$'$) now becomes (with $P_{-1}(z)$ interpreted as 0):

$$a_n P_{n+1}(z) + (b_n - z) P_n(z) + a_{n-1} P_{n-1}(z) = 0, \qquad n \geq 0 \tag{1.17}$$

so $P_n(z)$ obeys a second-order difference equation. If, for example, $\pi(x_0) \in \ell^2$, then x_0 is formally an eigenvalue of the Jacobi matrix A. (Of course, π is never a finite sequence because it obeys a second-order difference equation and $\pi_0(z) = 1$. Thus, $\pi \notin D(A)$. It may or may not happen that $\pi \in D(\bar{A})$, so the formal relation may or may not correspond to an actual eigenvalue. It will always be true, though, as we shall see, that if $\pi(x_0) \in \ell^2$, then $(A^* - x_0)\pi(x_0) = 0$.)

For convenience, set $a_{-1} = 1$. For any $z \in \mathbb{C}$, the solutions of the equation

$$a_n u_{n+1} + (b_n - z) u_n + a_{n-1} u_{n-1} = 0, \qquad n \geq 0 \tag{1.18}$$

are two-dimensional, determined by the initial data (u_{-1}, u_0).

$P_n(z)$ corresponds to taking

$$u_{-1} = 0, \qquad u_0 = 1.$$

There is a second solution, $Q_n(z)$, taking initial conditions

$$u_{-1} = -1, \qquad u_0 = 0.$$

We will also define $\xi(z) = (Q_0(z), Q_1(z), \dots)$. It can be seen by induction that for $n \geq 1$, $Q_n(X)$ is a polynomial of degree $n-1$. We will see later (Proposition 5.16) that the Q's are orthogonal polynomials for another moment problem.

As we will see, this normalization is such that if some combination $\eta(z) \equiv t\pi(z)+\xi(z) \in \ell^2$, then $(A^* - z)\eta = \delta_0$ and $\langle \delta_0, \eta \rangle = t$. Here δ_n is the Kronecker vector with 1 in position n and zeros elsewhere. We will have a lot more to say about $Q_n(z)$ in Section 4.

There is a fundamental result relating the solution vectors π, ξ to determinacy of the moment problem. In Section 4 (see Proposition 4.4 and Theorem 4.7), we will prove

Theorem 3. *Fix a set of moments and associated Jacobi matrix. Then the following are equivalent:*

(i) *The Hamburger moment problem is indeterminate.*
(ii) *For some $z_0 \in \mathbb{C}$ with $\operatorname{Im} z_0 \neq 0$, $\pi(z_0) \in \ell_2$.*
(iii) *For some $z_0 \in \mathbb{C}$ with $\operatorname{Im} z_0 \neq 0$, $\xi(z_0) \in \ell_2$.*
(iv) *For some $x_0 \in \mathbb{R}$, both $\pi(x_0)$ and $\xi(x_0)$ lie in ℓ_2.*
(v) *For some $x_0 \in \mathbb{R}$, both $\pi(x_0)$ and $\frac{\partial \pi}{\partial x}(x_0)$ lie in ℓ_2.*
(vi) *For some $x_0 \in \mathbb{R}$, both $\xi(x_0)$ and $\frac{\partial \xi}{\partial x}(x_0)$ lie in ℓ_2.*
(vii) *For all $z \in \mathbb{C}$, both $\pi(z)$ and $\xi(z)$ lie in ℓ_2.*

Remarks. 1. Appendix A has explicit determinantal formulae for $\sum_{n=0}^N |P_n(0)|^2$ and $\sum_{n=0}^N |Q_n(0)|^2$ providing "explicit" criteria for determinacy in terms of limits of determinants.

2. Theorem 3 can be thought of as a discrete analog of Weyl's limit point/limit circle theory for self-adjoint extensions of differential operators; see [34].

This implies that if all solutions of (1.18) lie in ℓ^2 for one $z \in \mathbb{C}$, then all solutions lie in ℓ^2 for all $z \in \mathbb{C}$.

A high point of the theory, discussed in Section 4, is an explicit description of all solutions of the moment problem in the indeterminate case in terms of a certain 2×2 matrix valued entire analytic function. It will suffice to only vaguely describe the full result in this introduction.

Definition. A *Herglotz function* is a function $\Phi(z)$ defined in $\mathbb{C}_+ \equiv \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}$ and analytic there with $\operatorname{Im} \Phi(z) > 0$ there.

These are also sometimes called Nevanlinna functions. It is a fundamental result (see, e.g., [2]) that given such a Φ, there exists $c \geq 0$, d real, and a measure $d\mu$ on $\mathbb{R}$ with $\int \frac{d\mu(x)}{1+x^2} < \infty$ so that either $c \neq 0$ or $d\mu \neq 0$ or both, and

$$\Phi(z) = cz + d + \int \left[\frac{1}{x-z} - \frac{x}{1+x^2} \right] d\mu(x). \tag{1.19}$$

Theorem 4. *The solutions of the Hamburger moment problem in the indeterminate case are naturally parametrized by Herglotz functions together with the functions* $\Phi(z) = t \in \mathbb{R} \cup \{\infty\}$*. This later set of solutions are the von Neumann solutions.*

If the Stieltjes problem is also indeterminate, there is $t_0 > 0$ *so that the solutions of the Stieltjes problem are naturally parametrized by Herglotz functions,* $\Phi(z)$*, which obey* $\Phi(x+i0) \in (t_0, \infty)$ *for* $x \in (-\infty, 0)$ *together with* $[t_0, \infty) \cup \{\infty\}$*. The later set of solutions are the von Neumann solutions.*

We will prove Theorem 4 in Section 4 (see Theorems 4.14 and 4.18). From the explicit Nevanlinna form of the solutions, one can prove (and we will in Section 4; see Theorems 4.11 and 4.17)

Theorem 5. *In the indeterminate case, the von Neumann solutions are all pure point measures. Moreover, for any* $t \in \mathbb{R}$*, there exists exactly one von Neumann solution,* $\mu^{(t)}$*, with* $\mu^{(t)}(\{t\}) > 0$*. Moreover, for any other solutions,* ρ*, of the moment problem,* $\rho(\{t\}) < \mu^{(t)}(\{t\})$*.*

Remark. The parametrization $\mu^{(t)}$ of this theorem is inconvenient since $t \mapsto \mu^{(t)}$ is many to one (in fact, infinity to one since each $\mu^{(t)}$ has infinite support). We will instead use a parametrization $t \mapsto \mu_t$ given by

$$\int \frac{d\mu_t(x)}{x} = t,$$

which we will see is a one-one map of $\mathbb{R} \cup \{\infty\}$ to the von Neumann solutions.

Examples 1.1 and 1.2 revisited. As noted, the explicit non-unique measures we listed were absolutely continuous measures. But there are, of necessity, many pure point measures that lead to the same moments. Indeed, the measures μ_t associated to the von Neumann solutions are each pure point. As we will see, there are many other pure point measures with the given moments. If ν is a Cantor measure, then it can be proven that $\int \mu_t \, d\nu(t)$ will be a singular continuous measure with the given moments. In the indeterminate case, the class of measures solving (1.1) is always extremely rich.

Given a set of moments $\{\gamma_n\}_{n=0}^\infty$ and $c \in \mathbb{R}$, one can define a new set of moments

$$\gamma_n(c) = \sum_{j=0}^{n} \binom{n}{j} c^j \gamma_{n-j}. \tag{1.20}$$

For the Hamburger problem, the solutions of the $\{\gamma_n\}_{n=0}^\infty$ and each $\{\gamma_n(c)\}_{n=0}^\infty$ problem are in one-one correspondence. If μ solves the $\{\gamma_n\}_{n=0}^\infty$ problem, then $d\rho(x-c) = d\rho_c(x)$ solves the $\{\gamma_n(c)\}_{n=0}^\infty$ problem, and vice-versa. But translation does not preserve the condition $\operatorname{supp}(\rho) \subset [0, \infty)$, so that as c decreases, the set of solutions of the Stieltjes problem shrinks. We will show that for any indeterminate Stieltjes moment problem, there is always a c_0, so that for $c > c_0$, $\{\gamma_n(c)\}_{n=0}^\infty$ is an indeterminate Stieltjes problem. For $c < c_0$, $\{\gamma_n(c)\}_{n=0}^\infty$ has no solution $d\rho$ with $\operatorname{supp}(d\rho) \subset [0, \infty)$, and $\{\gamma_n(c_0)\}$ is a

determinate Stieltjes problem (but, of course, an indeterminate Hamburger problem). This means there are lots of examples of moments which are determinate Stieltjes but indeterminate Hamburger. The existence of c_0 is intimately connected to Theorem 5. Among all the von Neumann solutions, there is a distinguished one, $d\mu_F$ (the Friedrichs solution), with $f_0 = \inf(\operatorname{supp}(\mu_t))$ maximal. One just takes $c_0 = -f_0$. That f_0 is a pure point of $d\mu_F$ is important in the analysis.

Another topic in the moment problem concerns the theory of Padé approximants, or what is esssentially the same thing — continued fractions. Typical is Theorem 6 below, which we will prove in Section 5.

Consider a sequence of numbers $\{\kappa_n\}_{n=0}^\infty$,

$$\kappa_n = (-1)^n \int_0^\infty x^n \, d\rho(x)$$

for some ρ. We are interested in "summing" the formal series (called a *series of Stieltjes*)

$$\sum_{n=0}^\infty \kappa_n z^n, \tag{1.21}$$

which is formally

$$\int_0^\infty \frac{d\rho(x)}{1+xz}\,. \tag{1.22}$$

If the series (1.21) converges, then (1.22) is analytic in a circle, $|z| < R$, which implies that ρ is supported in $[0, \frac{1}{R}]$. Thus, if $d\rho$ does not have compact support, then the series (1.21) will not converge for any $z \neq 0$.

Definition. The $[N, M]$ Padé approximant to the series (1.21) is the unique rational function of the form

$$f^{[N,M]}(z) \equiv \frac{A^{[N,M]}(z)}{B^{[N,M]}(z)}\,, \tag{1.23}$$

where A is a polynomial of degree N and B is a polynomial of degree M, and (as $z \to 0$)

$$f^{[N,M]}(z) - \sum_{n=0}^{N+M} \kappa_n z^n = O(z^{N+M+1}). \tag{1.24}$$

Note that A/B has $(N+1)+(M+1)-1 = N+M+1$ free parameters and $\{\kappa_n\}_{n=0}^{N+M}$ is $N+M+1$ free numbers. There is an explicit solution for A, B in terms of determinants; see Baker and Graves-Morris [4]. We will say more about the definition of Padé approximants in Section 5.

Theorem 6. *Let $\sum \kappa_n z^n$ be a series of Stieltjes. Then for any $z \in \mathbb{C}\backslash(-\infty,0)$, $\lim_{N\to\infty} f^{[N-1,N]}(z) \equiv f_-(z)$ exists and $\lim_{N\to\infty} f^{[N,N]}(z) = f_+(z)$ exists. The convergence is uniform on compact subsets of $\mathbb{C}\backslash(-\infty,0]$. Moreover, $f_+ = f_-$ if and only if the associated Stieltjes problem is determinate. If the problem is indeterminate and ρ is any solution of the associated Stieltjes problem, then*

$$f_-(x) \leq \int_0^\infty \frac{d\rho(y)}{1+xy} \leq f_+(x) \tag{1.25}$$

for any $x \in [0,\infty)$. In any event, for $x > 0$, $f^{[N,N]}(x)$ is monotone decreasing in N and $f^{[N-1,N]}(x)$ is monotone increasing.

In terms of the language of Section 3, f_- is associated to the Friedrichs solution and f_+ to the Krein solution. For an interesting application of Theorem 6, see [22, 36]. In Section 5, we will also discuss series of Hamburger and prove the new result that the $f^{[N,N]}(z)$ Padé approximants always converge in that case.

As a by-product of the proof of Theorem 6, we will find

Theorem 7. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Stieltjes moments. Then the Stieltjes problem is indeterminate if and only if*

$$\sum_{n=0}^\infty |P_n(0)|^2 < \infty \tag{1.26}$$

and

$$\sup_n \left| \frac{Q_n(0)}{P_n(0)} \right| < \infty. \tag{1.27}$$

Theorem 8. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Stieltjes moments. Then the Stieltjes problem is determinate while the Hamburger problem is indeterminate if and only if*

$$\sum_{n=0}^\infty |Q_n(0)|^2 < \infty \tag{1.28}$$

and

$$\lim_{n\to\infty} \left| \frac{Q_n(0)}{P_n(0)} \right| = \infty. \tag{1.29}$$

We will see that (1.26)/(1.27) are equivalent to a criterion of Stieltjes.

Theorem 6 is proven in Section 5 as parts of Theorem 5.2, Proposition 5.6, Proposition 5.8, and Proposition 5.11. Theorem 7 is Theorem 5.21 and Theorem 8 is Proposition 5.22.

In Section 6, which synthesizes and extends results in Akhiezer [1], we will study when the closure of the polynomials has finite codimension, and among our results proven as part of Theorem 6.4 is

Theorem 9. *Let ρ lie in $\mathcal{M}^H(\gamma)$ and let $\mathcal{H}_0$ be the closure of the set of polynomials in $\mathcal{H}_\rho \equiv L^2(\mathbb{R}, d\rho)$. Then $\mathcal{H}_0^\perp$ has finite dimension if and only if the Herglotz function, Φ, in the Nevanlinna parametrization of Theorem 4 is a real rational function* (*i.e., a ratio of real poynomials*)*. Equivalently, if and only if the measure μ of* (1.19) *has finite support.*

In fact, we will see that $\dim(\mathcal{H}_0^\perp)$ is the degree of the rational function Φ.

One consequence of this will be the following, proven in Appendix B (see Theorems B.1 and B.4).

Theorem 10. *$\mathcal{M}^H(\gamma)$ is a compact convex set* (*in the weak topology as a subset of the dual of $C(\mathbb{R} \cup \{\infty\})$*)*. Its extreme points are dense in the set.*

Remark. Do not confuse this density with the fact that the Krein-Millman theorem says that the convex combinations of the extreme points are dense. Here we have density without convex combinations, to be compared with the fact that in many other cases (e.g., probability measures on a compact Hausdorff space), the extreme points are closed.

Here is a sketch of the contents of the rest of this paper. In Section 2, we review von Neumann's theory of self-adjoint extensions and use it to prove the uniqueness result (Theorem 2) in the Hamburger case. In Section 3, we review the Birman-Krein-Vishik theory of semi-bounded self-adjoint extensions and use it to prove the uniqueness result (Theorem 3) in the Stieltjes case. In Section 4, we turn to a detailed analysis of the polynomials P and Q in terms of transfer matrices for the difference equation associated to the Jacobi matrix and prove Theorems 3, 4, and 5. In Section 5, we discuss Padé approximations and prove Theorems 6, 7, and 8. In Section 6, we discuss solutions, ρ, where the closure of the polynomials has finite codimension in $L^2(\mathbb{R}, d\rho)$. Appendix A is devoted to a variety of explicit formulae in terms of determinants of moments, and Appendix B to the structure of $\mathcal{M}^H(\gamma)$ as a compact convex set. Appendix C summarizes notation and some constructions.

§2. The Hamburger Moment Problem as a Self-Adjointness Problem

Let us begin this section with a brief review of the von Neumann theory of self-adjoint extensions. For further details, see [2, 5, 33, 34]. We start out with a densely defined operator A on a Hilbert space $\mathcal{H}$, that is, $D(A)$ is a dense subset of $\mathcal{H}$ and $A : D(A) \to \mathcal{H}$ a linear map. We will often consider its graph $\Gamma(A) \subset \mathcal{H} \times \mathcal{H}$ given by $\Gamma(A) = \{(\varphi, A\varphi) \mid \varphi \in D(A)\}$. Given operators A, B, we write $A \subset B$ and say B is an *extension* of A if and only if $\Gamma(A) \subset \Gamma(B)$.

One defines a new operator A^* as follows: $\eta \in D(A^*)$ if and only if there is a $\psi \in \mathcal{H}$ so that for all $\varphi \in D(A)$, $\langle \psi, \varphi \rangle = \langle \eta, A\varphi \rangle$. We set $A^*\eta = \psi$. In essence, A^*, called the *adjoint* of A, is the maximal object obeying

$$\langle A^*\eta, \varphi \rangle = \langle \eta, A\varphi \rangle \tag{2.1}$$

for all $\eta \in D(A^*)$, $\varphi \in D(A)$.

An operator is called *closed* if and only if $\Gamma(A)$ is a closed subset of $\mathcal{H}\times\mathcal{H}$ and it is called *closable* if and only if $\overline{\Gamma(A)}$ is the graph of an operator, in which case we define $\bar{A}$, the *closure* of A, by $\Gamma(\bar{A}) = \overline{\Gamma(A)}$. Thus, $D(\bar{A}) = \{\varphi\in\mathcal{H} \mid \exists\varphi_n\in D(A),$ so that $\varphi_n\to\varphi$ and $A\varphi_n$ is Cauchy$\}$ and one sets $A\varphi = \lim A\varphi_n$.

Adjoints are easily seen to be related to these notions: A^* is always closed; indeed,

$$\Gamma(A^*) = \{(A\varphi, -\varphi)\in\mathcal{H}\times\mathcal{H} \mid \varphi\in D(A)\}^\perp. \tag{2.2}$$

A^* is densely defined if and only if A is closable, in which case (by (2.2)), $\bar{A} = (A^*)^*$.

An operator is called *symmetric* if $A\subset A^*$ (equivalently, if $\langle\varphi, A\psi\rangle = \langle A\varphi,\psi\rangle$ for all $\varphi,\psi\in D(A)$), *self-adjoint* if $A = A^*$, and *essentially self-adjoint* if $\bar{A}$ is self-adjoint (equivalently, if A^* is self-adjoint). Notice that symmetric operators are always closable since $D(A^*)\supset D(A)$ is dense. Note also that if A is symmetric, then A^* is symmetric if and only if A is essentially self-adjoint.

Von Neumann's theory solves the following fundamental question: Given a symmetric operator A, when does it have self-adjoint extensions, are they unique, and how can they be described? If B is a self-adjoint extension of A, then B is closed, so $\bar{A}\subset B$. Thus, looking at self-adjoint extensions of A is the same as looking at self-adjoint extensions of $\bar{A}$. So for now, we will suppose A is a closed symmetric operator.

Define $\mathcal{K}_\pm = \ker(A^*\mp i)$, that is, $\mathcal{K}_+ = \{\varphi\in\mathcal{H} \mid A^*\varphi = i\varphi\}$. They are called the *deficiency subspaces*. Using $\|(A\pm i)\varphi\|^2 = \|A\varphi\|^2 + \|\varphi\|^2$, it is easy to see that if A is closed, then $\operatorname{Ran}(A\pm i)$ are closed, and since $\ker(A^*\mp i) = \operatorname{Ran}(A\pm i)^\perp$, we have

$$\operatorname{Ran}(A\pm i) = \mathcal{K}_\pm^\perp. \tag{2.3}$$

Let $d_\pm = \dim(\mathcal{K}_\pm)$, the *deficiency indices* of A.

Place the graph norm on $D(A^*)$, that is, $\|\varphi\|_{A^*}^2 = \langle\varphi,\varphi\rangle + \langle A^*\varphi, A^*\varphi\rangle$. This norm comes from an inner product, $\langle\varphi,\psi\rangle_{A^*} = \langle\varphi,\psi\rangle + \langle A^*\varphi, A^*\psi\rangle$.

Proposition 2.1. *Let A be a closed symmetric operator. Then*

$$D(A^*) = D(A)\oplus\mathcal{K}_+\oplus\mathcal{K}_-, \tag{2.4}$$

where $\oplus$ means orthogonal direct sum in the $\langle\,\cdot\,,\,\cdot\,\rangle_{A^*}$ inner product.

Proof. If $\varphi\in\mathcal{K}_+$ and $\psi\in\mathcal{K}_-$, then $\langle\varphi,\psi\rangle_{A^*} = \langle\varphi,\psi\rangle + \langle i\varphi, -i\psi\rangle = 0$ so $\mathcal{K}_+\perp_{A^*}\mathcal{K}_-$. If $\varphi\in D(A)$ and $\psi\in\mathcal{K}_\pm$, then $\langle A^*\varphi, A^*\psi\rangle = \langle A\varphi, \pm i\psi\rangle = \langle\varphi, \pm iA^*\psi\rangle = -\langle\varphi,\psi\rangle$, so $D(A)\perp_{A^*}\mathcal{K}_+\oplus\mathcal{K}_-$.

Let $\eta\in D(A^*)$. By (2.3), $\operatorname{Ran}(A+i)+\mathcal{K}_+ = \mathcal{H}$ so we can find $\varphi\in D(A)$ and $\psi\in\mathcal{K}_+$, so $(A^*+i)\eta = (A+i)\varphi + 2i\psi$. But then $(A^*+i)[\eta-\varphi-\psi] = 0$, so $\eta-\varphi-\psi\in\mathcal{K}_-$, that is, $\eta\in D(A)+\mathcal{K}_+ +\mathcal{K}_-$. $\square$

Corollary 2.2. (i) *Let A be a closed symmetric operator. Then A is self-adjoint if and only if $d_+ = d_- = 0$.*

(ii) *Let A be a symmetric operator. Then A is essentially self-adjoint if and only if $d_+ = d_- = 0$.*

If $A \subset B$, then $B^* \subset A^*$, so if B is symmetric, then $A \subset B \subset B^* \subset A^*$. Thus, to look for symmetric extensions of A, we need only look for operators B with $A \subset B \subset A^*$, that is, for restriction of A^* to $D(B)$'s with $D(A) \subset D(B)$. By Proposition 2.1, every such $D(B)$ has the form $D(A) + S$ with $S \subset \mathcal{K}_+ + \mathcal{K}_-$. On $D(A^*) \times D(A^*)$, define the sesquilinear form (sesquilinear means linear in the second factor and anti-linear in the first)

$$Q(\varphi, \psi) = \langle \varphi, A^*\psi\rangle_{\mathcal{H}} - \langle A^*\varphi, \psi\rangle_{\mathcal{H}}.$$

Proposition 2.3. *Let A be a closed symmetric operator. Then*

(i) *The operators B with $A \subset B \subset A^*$ are in one-one correspondence with subspaces S of $\mathcal{K}_+ + \mathcal{K}_-$ under $D(B) = D(A) + S$.*
(ii) *B is symmetric if and only if $Q \restriction D(B) \times D(B) = 0$.*
(iii) *B is symmetric if and only if $Q \restriction S \times S = 0$.*
(iv) *B is closed if and only if S is closed in $\mathcal{K}_+ \oplus \mathcal{K}_-$ in $D(A^*)$ norm.*
(v) *$\varphi \in D(A^*)$ lies in $D(B^*)$ if and only if $Q(\varphi, \psi) = 0$ for all $\psi \in D(B)$.*
(vi) *Let $J : \mathcal{K}_+ \oplus \mathcal{K}_- \to \mathcal{K}_+ \oplus \mathcal{K}_-$ by $J(\varphi, \psi) = (\varphi, -\psi)$. If $D(B) = D(A) + S$, then $D(B^*) = D(A) + J[S]^\perp$, where $^\perp$ is in $\mathcal{K}_+ \oplus \mathcal{K}_-$ in the $D(A^*)$ norm.*
(vii) *$\mathcal{K}_+(B) = \mathcal{K}_+ \cap S^\perp$, $\mathcal{K}_-(B) = \mathcal{K}_- \cap S^\perp$ (with $^\perp$ in the $\langle\, ,\, \rangle_{A^*}$ inner product).*

Proof. We have already seen (i) holds and (ii) is obvious. (iii) holds since if $\varphi \in D(A)$ and $\psi \in D(A^*)$, then $Q(\varphi, \psi) = 0$ by definition of A^* and symmetry of A. Thus, if $\varphi_1, \varphi_2 \in D(A)$ and $\psi_1, \psi_2 \in S$, then $Q(\varphi_1 + \psi_1, \varphi_2 + \psi_2) = Q(\psi_1, \psi_2)$. (iv) is immediate if one notes that $\Gamma(B) = \Gamma(A) \oplus \{(\varphi, A^*\varphi) \mid \varphi \in S\}$ with $\oplus$ in $\mathcal{H} \times \mathcal{H}$ norm and that the $\mathcal{H} \times \mathcal{H}$ norm on $\{(\varphi, A^*\varphi) \mid \varphi \in S\}$ is just the $D(A^*)$ norm. (v) follows from the definition of adjoint.

To prove (vi), let $\eta = (\eta_1, \eta_2)$, $\varphi = (\varphi_1, \varphi_2) \in \mathcal{K}_+ \oplus \mathcal{K}_-$. Then, direct calculations show that

$$Q(\eta, \varphi) = 2i[\langle \eta_1, \varphi_1\rangle_{\mathcal{H}} - \langle \eta_2, \varphi_2\rangle_{\mathcal{H}}] \tag{2.5}$$

$$\langle \eta, \varphi\rangle_{A^*} = 2[\langle \eta_1, \varphi_1\rangle_{\mathcal{H}} + \langle \eta_2, \varphi_2\rangle_{\mathcal{H}}]. \tag{2.6}$$

Thus, $Q(\eta, \varphi) = 0$ if and only if $\eta \perp J\varphi$. (v) thus implies (vi).

To prove (vii), note that by (vi), $\mathcal{K}_\pm(B) = \mathcal{K}_\pm \cap D(B^*) = \mathcal{K}_\pm \cap J[S]^\perp = \mathcal{K}_\pm \cap S^\perp$ since $\varphi \in \mathcal{K}_\pm$ lies in $J[S]^\perp$ if and only if $J\varphi$ lies in $S^\perp$ if and only if φ lies in $S^\perp$ by $J\varphi = \pm\varphi$ if $\varphi \in \mathcal{K}_\pm$. $\square$

With these preliminaries out of the way, we can prove von Neumann's classification theorem:

Theorem 2.4. *Let A be a closed symmetric operator. The closed symmetric extensions B of A are in one-one correspondence with partial isometries of $\mathcal{K}_+$ into $\mathcal{K}_-$, that is, maps $U : \mathcal{K}_+ \to \mathcal{K}_-$ for which there are closed subspaces $\mathcal{U}_+ \subset \mathcal{K}_+$ and $\mathcal{U}_- \subset \mathcal{K}_-$ so that U is a unitary map of $\mathcal{U}_+ \to \mathcal{U}_-$ and $U \equiv 0$ on $\mathcal{U}_+^\perp$. If B corresponds to U, then $D(B) = D(A) + \{\varphi + U\varphi \mid \varphi \in \mathcal{U}_+\}$. Moreover, $\mathcal{K}_\pm(B) = \mathcal{K}_\pm \cap \mathcal{U}_\pm^\perp$ ($\mathcal{H}$ orthogonal complement). In particular, A has self-adjoint extensions if and only if $d_+ = d_-$ and then the self-adjoint extensions are in one-one correspondence with unitary maps U from $\mathcal{K}_+$ to $\mathcal{K}_-$.*

Proof. Let B be a symmetric extension of A. Let $\varphi \in D(B) \cap (\mathcal{K}_+ \oplus \mathcal{K}_-)$, say $\varphi = (\varphi_1 + \varphi_2)$. By (2.5), $Q(\varphi, \varphi) = 2i(\|\varphi_1\|^2 - \|\varphi_2\|^2)$, so B symmetric implies that $\|\varphi_1\| = \|\varphi_2\|$, so $D(B) \cap (\mathcal{K}_+ \oplus \mathcal{K}_-) = \{\text{some } (\varphi_1, \varphi_2)\}$, where $\|\varphi_1\| = \|\varphi_2\|$. Since $D(B)$ is a subspace, one cannot have (φ_1, φ_2) and (φ_1, φ_2') with $\varphi_2 \neq \varphi_2'$ (for then $(0, \varphi_2 - \varphi_2') \in D(B)$ so $\|\varphi_2 - \varphi_2'\| = 0$). Thus, $D(B) \cap (\mathcal{K}_+ \oplus \mathcal{K}_-)$ is the graph of a partial isometry. On the other hand, if U is a partial isometry, $Q(\varphi + U\varphi, \psi + U\psi) = 2i(\langle \varphi, \psi \rangle - \langle U\varphi, U\psi \rangle) = 0$ so each U does yield a symmetric extension.

That $\mathcal{K}_\pm(B) = \mathcal{K}_\pm \cap \mathcal{U}_\pm^\perp$ follows from (vii) of the last proposition if we note that if $\varphi \in \mathcal{K}_+$, then $\varphi \perp_{A^*} \{(\psi + U\psi) \mid \psi \in \mathcal{U}_+\}$ if and only if $\varphi \perp_{A^*} \{\psi \mid \psi \in \mathcal{U}_+\}$ if and only if $\varphi \perp_{\mathcal{H}} \mathcal{U}_+$ (by (2.6)).

Thus B is self-adjoint if and only if U is a unitary from $\mathcal{K}_+$ to $\mathcal{K}_-$, which completes the proof. $\square$

Recall that a map T is *anti-linear* if $T(a\varphi + b\psi) = \bar{a}T(\varphi) + \bar{b}T(\psi)$ for $a, b \in \mathbb{C}$, $\varphi, \psi \in \mathcal{H}$; that T is *anti-unitary* if it is anti-linear, a bijection, and norm-preserving; and that a *complex conjugation* is an anti-unitary map whose sequence is 1.

Corollary 2.5. *Let A be a symmetric operator. Suppose there exists a complex conjugation $C : \mathcal{H} \to \mathcal{H}$ so that $C : D(A) \to D(A)$ and $CA\varphi = AC\varphi$ for all $\varphi \in D(A)$. Then A has self-adjoint extensions. If $d_+ = 1$, every self-adjoint extension B is real, that is, obeys $C : D(B) \to D(B)$ and $CB\varphi = BC\varphi$ for all $\varphi \in D(B)$. If $d_+ \geq 2$, there are non-real self-adjoint extensions.*

Proof. C is an anti-unitary from $\mathcal{K}_+$ to $\mathcal{K}_-$ so $d_+ = d_-$.

We claim that if B is self-adjoint and is associated to $U : \mathcal{K}_+ \to \mathcal{K}_-$, then B is real if and only if $CUCU = 1$ for it is easy to see that $C : D(A^*) \to D(A^*)$ and $CA^*\varphi = A^*C\varphi$, so B is real if and only if C maps $D(B)$ to itself. Thus, $C(\varphi + U\varphi)$ must be of the form $\psi + U\psi$. Since ψ must be $CU\varphi$, this happens if and only if $C\varphi = UCU\varphi$, that is, $CUCU\varphi = \varphi$. This proves our claim.

If $d_+ = 1$ and $\varphi \in \mathcal{K}_+$, $CU\varphi = e^{i\theta}\varphi$ for some θ. Then $(CUCU)\varphi = Ce^{i\theta}U\varphi = e^{-i\theta}CU\varphi = \varphi$ showing that every self-adjoint extension is real.

If $d_+ \geq 2$, pick $\varphi, \psi \in \mathcal{K}_+$ with $\varphi \perp \psi$ and let $U\varphi = C\psi$, $U\psi = iC\varphi$. Then $CUCU\varphi = CUCC\psi = CU\psi = CiC\psi = -i\varphi$, so $CUCU \not\equiv 1$. Thus, the B associated to this U will not be real. $\square$

Next we analyze a special situation that will always apply to indeterminate Hamburger moment problems.

Theorem 2.6. *Suppose that A is a closed symmetric operator so that there exists a complex conjugation under which A is real. Suppose that $d_+ = 1$ and that* $\ker(A) = \{0\}$, $\dim\ker(A^*) = 1$. *Pick $\varphi \in \ker(A^*)$, $C\varphi = \varphi$, and $\eta \in D(A^*)$, not in $D(A) + \ker(A^*)$. Then $\langle \varphi, A^*\eta\rangle \neq 0$ and $\psi = \{\eta - [\langle \eta, A^*\eta\rangle / \langle \varphi, A^*\eta\rangle]\varphi\}/\langle \varphi, A^*\eta\rangle$ are such that in φ, ψ basis, $\langle\,\cdot\,, A^*\,\cdot\,\rangle$ has the form*

$$\langle\,\cdot\,, A^*\,\cdot\,\rangle = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}. \tag{2.7}$$

The self-adjoint extensions, B_t, can be labelled by a real number or ∞ where

$$\begin{aligned} D(B_t) &= D(A) + \{\alpha(t\varphi + \psi) \mid \alpha \in \mathbb{C}\} && t \in \mathbb{R} \\ &= D(A) + \{\alpha\varphi \mid \alpha \in \mathbb{C}\} && t = \infty. \end{aligned}$$

The operators B_t are independent of which real ψ in $D(A^*)\backslash D(A)$ is chosen so that (2.7) *holds.*

Proof. If $\langle \varphi, A^*\eta\rangle = 0$, then the $\langle\,\cdot\,, A^*\,\cdot\,\rangle$ matrix with basis φ, η would have the form $\left(\begin{smallmatrix} a & 0 \\ 0 & 0 \end{smallmatrix}\right)$ with $a \in \mathbb{R}$, in which case $Q \equiv 0$ on the span of φ and η, which is incompatible with the fact that $d_+ = 1$. Thus, $\langle \varphi, A^*\eta\rangle \neq 0$ and (2.7) holds by an elementary calculation.

Once (2.7) holds, it is easy to see that the subspaces S of $D(A^*)$ with $D(A) \subset S$, $\dim(S/D(A)) = 1$, and $Q \restriction S \times S = 0$ are precisely the $D(B_t)$.

If $\tilde{\psi}$ is a second ψ for which (2.7) holds, then $Q(\psi - \tilde{\psi}, \rho) = 0$ for all $\rho \in D(A^*)$, so $\psi - \tilde{\psi} \in D(A)$ and the $D(B_t)$'s are the same for ψ and $\tilde{\psi}$. $\square$

Remarks. 1. It is easy to see that if $\ker(A) = \{0\}$, then $\dim\ker(A^*) \leq d_+$, so if $d_+ = 1$ and $\ker(A) = \{0\}$, $\dim\ker(A^*)$ is either 0 or 1. The example of $A = -\frac{d^2}{dx^2}$ on $L^2(0,\infty)$ with $D(A) = C_0^\infty(0,\infty)$ shows that it can happen that A is real, $d_+ = 1$, but $\dim\ker(A^*) = 0$.

2. One example where this formalism is natural is if $A \geq \alpha > 0$ (for $\alpha \in \mathbb{R}$), in which case $\dim\ker(A^*) = d_+$. One takes $\eta = A_F^{-1}\varphi$, where A_F is the Friedrichs extension. We will discuss this further in Section 3. A second example, as we will see, is the indeterminate moment problem, in which case one can take $\varphi = \pi(0)$, $\psi = \xi(0)$.

We can now turn to the analysis of the symmetric operator A on $\mathcal{H}^{(\gamma)}$ described in Section 1. In terms of the explicit basis $P_n(X)$ in $\mathcal{H}^{(\gamma)}$, we know A has the Jacobi matrix form (1.16). We will first explicitly describe A^* and the form Q. Given any sequence $s = (s_0, s_1, \dots)$, we define a new sequence $\mathcal{F}(s)$ (think of $\mathcal{F}$ for "formal adjoint") by

$$\mathcal{F}(s)_n = \begin{cases} b_0 s_0 + a_0 s_1 & \text{if } n = 0 \\ a_{n-1}s_{n-1} + b_n s_n + a_n s_{n+1} & \text{if } n \geq 1. \end{cases}$$

Given any two sequences, s_n and t_n, we define their Wronskian,

$$W(s,t)(n) = a_n(s_{n+1}t_n - s_n t_{n+1}). \tag{2.8}$$

The Wronskian has the following standard property if

$$a_n s_{n+1} + c_n s_n + a_{n-1} s_{n-1} = 0 \tag{2.9}$$

and

$$a_n t_{n+1} + d_n t_n + a_{n-1} t_{n-1} = 0. \tag{2.10}$$

Then multiplying (2.9) by t_n and subtracting (2.10) multiplied by s_n, we see that

$$W(s,t)(n) - W(s,t)(n-1) = (d_n - c_n) s_n t_n. \tag{2.11}$$

In particular, if $d = c$, then W is constant.

Theorem 2.7. *Let A be the Jacobi matrix* (1.16) *with $D(A) = \{s \mid s_n = 0$ for n sufficiently large$\}$. Then*

$$D(A^*) = \{s \in \ell_2 \mid \mathcal{F}(s) \in \ell_2\} \tag{2.12}$$

with

$$A^* s = \mathcal{F}(s) \tag{2.13}$$

for $s \in D(A^*)$. Moreover, if $s, t \in D(A^*)$, then

$$\lim_{n\to\infty} W(\bar{s}, t)(n) = \langle A^* s, t\rangle - \langle s, A^* t\rangle. \tag{2.14}$$

Proof. Since the matrix (1.16) is a real-symmetric matrix, it is easy to see that for any $t \in D(A)$, and any sequences

$$\langle s, At\rangle = \langle \mathcal{F}(s), t\rangle. \tag{2.15}$$

Since t and At are finite sequences, the sum in $\langle\,\cdot\,,\,\cdot\,\rangle$ makes sense even if s or $\mathcal{F}(s)$ are not in ℓ_2. Since $D(A)$ is dense in ℓ_2, (2.15) says that $s \in \ell_2$ lies in $D(A^*)$ precisely if $\mathcal{F}(s) \in \ell_2$ and then (2.13) holds. That proves the first part of the theorem.

For the second, we perform a calculation identical to that leading to (2.11):

$$\begin{aligned}\sum_{n=0}^{N} \left[\,\overline{\mathcal{F}s_n}\, t_n - \overline{s_n}\,(\mathcal{F}t_n)\right] &= W(\bar{s},t)(0) + \sum_{n=1}^{N} W(\bar{s},t)(n) - W(\bar{s},t)(n-1) \\ &= W(\bar{s},t)(N).\end{aligned} \tag{2.16}$$

If $s, t \in D(A^*)$, then the left side of (2.16) converges to $\langle A^* s, t\rangle - \langle s, A^* t\rangle$ as $N \to \infty$, so (2.14) holds. $\square$

Lemma 2.8. *If $\varphi \in D(A^*)$, $(A^* - z)\varphi = 0$ for some z and $\varphi_0 = 0$, then $\varphi \equiv 0$.*

Proof. Essentially, this is so because $(A^* - z)s = 0$ is a second-order difference equation with $s_{-1} \equiv 0$, so solutions are determined by s_0. Explicitly, suppose $A^* s = zs$ and $s_0 = 0$. Then

$$\begin{aligned} s_{n+1} &= a_n^{-1}[(-b_n + z)s_n - a_{n-1}s_{n-1}], &\qquad n \geq 1 \\ &= a_0^{-1}[(-b_0 + z)s_0], & n = 0. \end{aligned}$$

By a simple induction, $s \equiv 0$. $\square$

Corollary 2.9. *The operator A associated to a Hamburger moment problem always has either deficiency indices $(1,1)$ or deficiency indices $(0,0)$.*

Proof. We have already seen that $d_+ = d_-$ so it suffices to show that $\ker(A^* - i)$ has dimension at most 1. By Lemma 2.8, the map from $\ker(A^* - i)$ to $\mathbb{C}$ that takes $s \mapsto s_0$ is one-one, so $\ker(A^* - i)$ is of dimension 0 or 1. $\square$

We are now ready to prove the more subtle half of the Hamburger part of Theorem 2.

Theorem 2.10 (one quarter of Theorem 2). *Let A be essentially self-adjoint. Then the Hamburger moment problem has a unique solution.*

Proof. Pick z with $\operatorname{Im} z > 0$ and a measure ρ obeying (1.1). Since A is essentially self-adjoint, $(A - i)[D(A)]$ is dense in ℓ^2, and by an identical argument, $(A - z)[D(A)]$ is dense in ℓ^2. Thus, there exists a sequence $R_n^{(z)}(X)$ of polynomials so that

$$\|(X - z)R_n^{(z)}(X) - 1\| \to 0$$

in $\mathcal{H}^{(\gamma)}$, and thus

$$\int [(x - z)R_n^{(z)}(x) - 1]^2 \, d\rho(x) \to 0$$

since $d\rho(x)$ realizes $\mathcal{H}^{(\gamma)}$ on polynomials. Now $\frac{1}{x-z}$ is bounded for $x \in \mathbb{R}$ since $\operatorname{Im} z > 0$. Thus

$$\int \left| R_n^{(z)}(x) - \frac{1}{x - z} \right|^2 d\rho(x) \to 0.$$

It follows that

$$G_\rho(x) \equiv \int \frac{d\rho(x)}{x - z} = \lim_{n\to\infty} \int R_n^{(z)}(x)\, d\rho(x)$$

is independent of ρ. Since $G_\rho(x)$ determines ρ (because $\rho(\{a\}) = \lim_{\varepsilon\downarrow 0} \varepsilon \operatorname{Im} G_\rho(a + i\varepsilon)$ and $\rho((a,b)) + \rho([a,b]) = \frac{2}{\pi} \lim_{\varepsilon\downarrow 0} \int_a^b \operatorname{Im} G_\rho(y + i\varepsilon)\, dy$), all ρ's must be the same. $\square$

Theorem 2.11. *Let A be a Jacobi matrix with $D(A)$ the sequences of finite support. Suppose A is not essentially self-adjoint and B, F are distinct self-adjoint extensions of A. Then*

$$\left(\delta_0, \frac{1}{B - i}\, \delta_0\right) \neq \left(\delta_0, \frac{1}{F - i}\, \delta_0\right). \tag{2.17}$$

Remarks. 1. The proof shows for any $z \in \mathbb{C}\backslash\mathbb{R}$, $(\delta_0, (B - z)^{-1}\delta_0) \neq (\delta_0 (F - z)^{-1}\delta_0)$. It also works for $z \in \mathbb{R}$ as long as z is in the resolvent set for both B and F.

2. In Section 4, we will have a lot more to say about the possible values of $(\delta_0, \frac{1}{B-z}\delta_0)$ as B runs through the self-adjoint extensions of A.

Proof. We first claim that $\delta_0 \notin \operatorname{Ran}(A - i)$. For suppose on the contrary that there exists $\eta \in D(A)$ and $\delta_0 = (A - i)\eta$ and that $(A^* + i)\varphi = 0$. Then $(\delta_0, \varphi) = ((A - i)\eta, \varphi) =$

$(\eta, (A^*+i)\varphi) = 0$. By Lemma 2.8, $\varphi \equiv 0$. Thus, if $\delta_0 \in \operatorname{Ran}(A-i)$, then $\ker(A^*+i) = \{0\}$, so A is essentially self-adjoint. By hypothesis, this is false, so $\delta_0 \notin \operatorname{Ran}(A-i)$.

Thus, $(B-i)^{-1}\delta_0$ and $(F-i)^{-1}\delta_0$ are in $D(A^*)\backslash D(A)$. Since $\dim(D(B)/D(A)) = \dim(D(F)/D(A)) = 1$, if these vectors were equal, $D(B)$ would equal $D(F)$, so $B = A^* \upharpoonright D(B)$ would equal $F = A^* \upharpoonright D(F)$. Thus, $(B-i)^{-1}\delta_0 \neq (F-i)^{-1}\delta_0$.

Let $\eta = (B-i)^{-1}\delta_0 - (F-i)^{-1}\delta_0$. Then

$$(A^*-i)\eta = (A^*-i)(B-i)^{-1}\delta_0 - (A^*-i)(F-i)^{-1}\delta_0 = \delta_0 - \delta_0 = 0,$$

so $\eta \neq 0$ implies $\eta_0 \neq 0$ by Lemma 2.8. Thus, $(\delta_0, \eta) = (\delta_0, (B-i)^{-1}\delta_0) - (\delta_0, (F-i)^{-1}\delta_0) \neq 0$. $\square$

As a corollary of Theorem 2.11, we have

Theorem 2.12 (two quarters of Theorem 2). *A Hamburger moment problem for which A is not essentially self-adjoint is indeterminate. A Stieltjes moment problem for which A has multiple non-negative self-adjoint extensions is indeterminate.*

Proof. Theorem 2.11 implies that distinct self-adjoint extensions lead to distinct spectral measures since

$$(\delta_0, (B-i)^{-1}\delta_0) = \int \frac{d\mu^B(x)}{x-i},$$

where μ^B is the solution to (1.1) associated to B. Positive self-adjoint extensions yield solutions of the Stieltjes moment problem. $\square$

With this machinery available, we can prove the converse of Proposition 1.6:

Theorem 2.13. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of moments for which the Stieltjes problem has solutions. Let*

$$\Gamma_{2m} = \gamma_m, \qquad m = 0, 1, \dots \tag{2.18a}$$

$$\Gamma_{2m+1} = 0, \qquad m = 0, 1, \dots. \tag{2.18b}$$

Then $\{\Gamma_j\}_{j=0}^\infty$ is a determinate Hamburger problem if and only if $\{\gamma_n\}_{n=0}^\infty$ is a determinate Stieltjes problem.

Proof. The proof of Proposition 1.6 shows there is a one-one correspondence between solutions of the Stieltjes problem for γ and those solutions $d\rho$ of the Hamburger problem for Γ with $d\rho(-x) = d\rho(x)$. We will call such solutions symmetric. Thus it suffices to show that if the Hamburger problem for Γ is indeterminate, then there are multiple symmetric solutions.

Let U map $\mathbb{C}(X)$ to itself by $U[P(X)] = P(-X)$. By $\Gamma_{2m+1} = 0$, U is unitary, and so extends to a unitary map from $\mathcal{H}^{(\Gamma)}$ to itself. Clearly, U maps $D(A) = \mathbb{C}(X)$ to itself and $UAU^{-1} = -A$.

Thus, U maps $D(A^*)$ to itself and $UA^*U^{-1} = -A^*$. This means that U maps $\mathcal{K}_+$ to $\mathcal{K}_-$.

Let C be the complex conjugation under which A is real. Then $UC = CU$ is an anti-unitary map of $\mathcal{K}_+$ to itself. So if φ is a unit vector in $\mathcal{K}_+$, then $UC\varphi = e^{i\theta}\varphi$ for some real θ. Thus, $UC(e^{i\theta/2}\varphi) = e^{-i\theta/2}UC\varphi = e^{i\theta/2}\varphi$ so there exists $\psi \neq 0$ in $\mathcal{K}_+$ with $UC\psi = \psi$.

In particular, since $UC = CU$, $U(\psi \pm C\psi) = \pm(\psi \pm C\psi)$ and therefore, if $B = A^* \restriction D(B)$ and $F = A^* \restriction D(F)$, where $D(B) = D(A) + [\psi + C\psi]$ and $D(F) = D(A) + [\psi - C\psi]$, then U leaves both $D(B)$ and $D(F)$ invariant, and so B and F are distinct extensions with $UBU^{-1} = -B$ and $UFU^{-1} = -F$. Their spectral measures thus yield distinct symmetric extensions. $\square$

Remark. Since $U(\psi + e^{i\theta}C\psi) = e^{i\theta}(\psi + e^{-i\theta}C\psi)$, we see that if $\theta \neq 0, \pi$, then U does not leave $D(B_\theta)$ invariant. Thus among von Neumann solutions of the Γ problem, exactly two are symmetric.

As a consequence of our identification of A^*, we can prove one small part of Theorem 3. Recall that $\pi(x_0)$ is the sequence $\{P_n(x_0)\}_{n=0}^\infty$ and $\xi(x_0)$ is the sequence $\{Q_n(x_0)\}_{n=i}^\infty$.

Theorem 2.14. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Hamburger moments. If either of the following holds, then the Hamburger moment problem is indeterminate.*

(i) *For some $x_0 \in \mathbb{R}$, $\pi(x_0)$ and $\frac{\partial\pi}{\partial x}(x_0)$ lie in ℓ_2.*
(ii) *For some $x_0 \in \mathbb{R}$, $\xi(x_0)$ and $\frac{\partial\xi}{\partial x}(x_0)$ lie in ℓ_2.*

Remark. Since $P_n(z)$ is a polynomial, $\frac{\partial\pi}{\partial x}$ makes sense as a sequence.

Proof. In terms of the formal adjoint $\mathcal{F}$, we have

$$\mathcal{F}(\pi(x_0)) = x_0\pi(x_0) \tag{2.19}$$

$$\mathcal{F}\biggl(\frac{\partial\pi}{\partial x}\,(x_0)\biggr) = \pi(x_0) + x_0\,\frac{\partial\pi}{\partial x}\,(x_0) \tag{2.20}$$

$$\mathcal{F}(\xi(x_0)) = \delta_0 + x_0\xi(x_0) \tag{2.21}$$

$$\mathcal{F}\biggl(\frac{\partial\xi}{\partial x}\,(x_0)\biggr) = \xi(x_0) + x_0\,\frac{\partial\xi}{\partial x_0}\,. \tag{2.22}$$

Thus, if (i) holds, we conclude π, $\frac{\partial\pi}{\partial x}$ are in $D(A^*)$ and

$$(A^* - x_0)\pi(x_0) = 0, \qquad (A^* - x_0)\frac{\partial\pi}{\partial x}\bigg|_{x=x_0} = \pi(x_0).$$

If A^* were self-adjoint, then

$$\|\pi(x_0)\|^2 = \biggl\langle\, \pi, (A^* - x_0)\frac{\partial\pi}{\partial x}\bigg|_{x=x_0} \biggr\rangle = \biggl\langle\, (A^* - x_0)\pi, \frac{\partial\pi}{\partial x}\bigg|_{x=x_0} \biggr\rangle = 0,$$

which is impossible since $P_0(x_0) = 1$. Thus, A^* is not self-adjoint and the problem is indeterminate.

If (ii) holds, $\xi, \frac{\partial \xi}{\partial x}$ are in $D(A^*)$ and

$$(A^* - x_0)\xi(x_0) = \delta_0, \qquad (A^* - x_0)\frac{\partial \xi}{\partial x}\bigg|_{x=x_0} = \xi(x_0).$$

If A^* were self-adjoint, then

$$\begin{aligned} \|\xi(x_0)\|^2 &= \left\langle \xi(x_0), (A^* - x_0)\frac{\partial \xi}{\partial x}\bigg|_{x=x_0} \right\rangle \\ &= \left\langle (A^* - x_0)\xi(x_0), \frac{\partial \xi}{\partial x}\bigg|_{x=x_0} \right\rangle \\ &= \frac{\partial Q_0(x)}{\partial x}\bigg|_{x=x_0} = 0 \end{aligned}$$

since $Q_0(x_0) \equiv 0$. This is impossible since $Q_1(x_0) \neq 0$ and so again, the problem is indeterminate. $\square$

While we have used the theory of essential self-adjointness to study the moment problem, following Nussbaum [30], one can turn the analysis around:

Definition. Let B be a symmetric operator on a Hilbert space $\mathcal{H}$ and let $\varphi \in C^\infty(B) = \cap_n D(B^n)$. φ is called *a vector of uniqueness for* B if and only if the Hamburger moment problem for

$$\gamma_n = \frac{(\varphi, B^n\varphi)}{\|\varphi\|^2} \tag{2.23}$$

is determinate.

Theorem 2.15 (Nussbaum [30]). *Let B be a (densely defined) symmetric operator on a Hilbert space $\mathcal{H}$. Suppose that $D(B)$ contains a dense subset of vectors of uniqueness. Then B is essentially self-adjoint.*

Proof. Let $\mathcal{U}$ be the vectors of uniqueness for B. Let $\varphi \in \mathcal{U}$ and let A_φ be the restriction of B to the closure of the space spanned by $\{B^n\varphi\}_{n=0}^\infty$. A_φ is unitarily equivalent to the Jacobi matrix for the moment problem (2.23). Thus, A_φ is essentially self-adjoint on $\mathcal{H}_\varphi$, the closure of the span of $\{B^n\varphi\}_{n=0}^\infty$. Therefore, $\overline{(A_\varphi + i)[D(A_\varphi)]} = \mathcal{H}_\varphi$ and, in particular, $\varphi \in \overline{(A_\varphi + i)[D(A_\varphi)]} \subset \overline{(B + i)[D(B)]}$. It follows that $\mathcal{U} \subset \overline{(B+i)[D(B)]}$ and thus, $\overline{\mathrm{Ran}(B + i)} = \mathcal{H}$. Similarly, $\overline{\mathrm{Ran}(B - i)} = \mathcal{H}$, so B is essentially self-adjoint by Corollary 2.2. $\square$

The motivation for Nussbaum was understanding a result of Nelson [28].

Definition. Let B be a symmetric operator. $\varphi \in C^\infty$ is called

analytic if $\|B^n\varphi\| \leq CR^n n!$
semi-analytic if $\|B^n\varphi\| \leq CR^n (2n)!$
quasi-analytic if $\sum_{n=1}^\infty \|B^{2n}\varphi\|^{1/2n} < \infty$.
Stieltjes if $\sum_{n=1}^\infty \|B^n\varphi\|^{1/2n} < \infty$.

Corollary 2.16. *If B is a symmetric operator, then any analytic or quasi-analytic vector is a vector of uniqueness. If B is also bounded from below, then any semi-analytic or Stieltjes vector is a vector of uniqueness. In particular,*

- (i) (Nelson [28]) *If $D(B)$ contains a dense set of analytic vectors, then B is essentially self-adjoint.*
- (ii) (Nussbaum [31], Masson-McClary [23]) *If $D(B)$ contains a dense set of semi-analytic vectors and is bounded from below, then B is essentially self-adjoint.*
- (iii) (Nussbaum [30]) *If $D(B)$ contains a dense set of quasi-analytic vectors, then B is essentially self-adjoint.*
- (iv) (Nussbaum [31], Masson-McClary [23]) *If $D(B)$ contains a dense set of Stieltjes vectors and is bounded from below, then B is essentially self-adjoint.*

Proof. The first two assertions follow Proposition 1.5, Corollary 3.4, and Corollary 4.5. Theorem 2.14 completes the proof. $\square$

§3. The Stieltjes Moment Problem as a Self-Adjointness Problem

One goal in this section is to prove the remaining part of Theorem 2, namely, that if the operator A has a unique non-negative self-adjoint extension, then the Stieltjes problem is determinate. In the indeterminate case, we will also introduce two distinguished non-negative von Neumann solutions: the Friedrichs and Krein solutions.

The name Friedrichs and Krein for the associated self-adjoint extensions is standard. We will naturally carry over the names to the measures $d\mu_F$ and $d\mu_K$ that solve the Stieltjes problem. Those names are not standard. Krein did important work on the moment problem, but not in the context of what we will call the Krein solution because of his work on self-adjoint extensions.

We begin with a very brief summary of the Birman-Krein-Vishik theory of extensions of strictly positive operators (see [3] for a complete exposition). Suppose A is a closed symmetric operator and for some $\alpha > 0$, $(\varphi, A\varphi) \geq \alpha\|\varphi\|^2$ for all $\varphi \in D(A)$. One closes the quadratic form analogously to closing the operator, that is, $\varphi \in Q(A_F)$ if and only if there is $\varphi_n \in D(A)$ so that $\varphi_n \to \varphi$ and $(\varphi_n - \varphi_m, A(\varphi_n - \varphi_m)) \to 0$ as $n \to \infty$. One then sets $(\varphi, A_F\varphi) = \lim(\varphi_n, A\varphi_n)$. The quadratic form $(\varphi, A_F\varphi)$ on $Q(A_F)$ is closed, that is, $Q(A_F)$ is complete in the norm $\sqrt{(\varphi, A_F\varphi)}$.

Not every quadratic form abstractly defined is closable (e.g., on $L^2(\mathbb{R}, dx)$, the form with form domain $C_0^\infty(\mathbb{R})$ given by $\varphi \mapsto |\varphi(0)|^2$ is not closable), but it is not hard to see that if a quadratic form comes from a non-negative symmetric operator, it is closable (see Theorem X.23 in [34] or [12], Chapter VI).

While a closed symmetric operator need not be self-adjoint, it is a deep result (see [12, 34]) that a closed positive quadratic form is always the quadratic form of a self-adjoint operator. It follows that A_F is the quadratic form of a self-adjoint operator, the *Friedrichs extension* of A. It follows that $\inf \operatorname{spec}(A_F) = \alpha > 0$.

Define $N = \ker(A^*)$ which is closed since A^* is a closed operator. Then $D(A^*) = D(A) + N + A_F^{-1}[N]$, where $+$ means independent sum. In particular, $N \neq \{0\}$ if A is

not self-adjoint (which we suppose in the rest of this paragraph). The *Krein extension* is the one with $D(A_K) = D(A) + N$. Then $Q(A_K) = Q(A_F) + N$. Since $N \subset D(A_K)$, we have that $\inf \operatorname{spec}(A_K) = 0$ so $A_K \neq A_F$. The set of non-negative self-adjoint extensions of A is precisely the set of self-adjoint operators B with $A_K \leq B \leq A_F$ (where $0 \leq C \leq D$ if and only if $Q(D) \subset Q(C)$ and $(\varphi, C\varphi) \leq (\varphi, D\varphi)$ for all $\varphi \in Q(D)$; equivalently, if and only if $(D+1)^{-1} \leq (C+1)^{-1}$ as bounded operators). These B's can be completely described in terms of closed but not necessarily densely defined quadratic forms, C, on N. One can think of $C = \infty$ on $Q(C)^{\perp}$. A_F corresponds to $C \equiv \infty$ (i.e., $Q(C) = \{0\}$) and A_K to $C \equiv 0$. In general, $Q(A_C) = Q(A_F) + Q(C)$ and if $\varphi \in Q(A_F)$ and $\eta \in Q(C)$, then $(\varphi + \eta, A_C(\varphi + \eta)) = (\varphi, A_F\varphi) + (\eta, C\eta)$.

Two aspects of Jacobi matrices (defined on sequences of finite support) make the theory special. First, $\dim(N) \leq 1$. Second, by Theorem 5 (which we will prove in the next section without using any results from the present section), if A is not essentially self-adjoint, A_F has a discrete spectrum with the property that if $t \in \operatorname{spec}(A_F)$, then $\mu_F(\{t\}) > \mu(\{t\})$ for any other solution, μ, of the Hamburger moment problem. Moreover, if $t \in \operatorname{spec}(A_F)$, $t \notin \operatorname{spec}(B)$ for any other self-adjoint extension, B.

Proposition 3.1. *Let A be a Jacobi matrix defined on the sequences of finite support, and suppose that A has deficiency indices* $(1,1)$ *and that A is non-negative* (*i.e., that the moment problem associated to A has at least some solutions of the Stieltjes moment problem*). *Then A has a unique non-negative self-adjoint extension if and only if* 0 *is an eigenvalue in the spectrum of A_F.*

Proof. Let $\alpha = \inf \operatorname{spec}(A_F)$. By hypothesis, $\alpha \geq 0$, and by Theorem 5, α is a discrete, simple eigenvalue of A_F. We want to show that if $\alpha > 0$, then A has additional non-negative self-adjoint extensions; and contrary-wise, if $\alpha = 0$, then it has no additional non-negative self-adjoint extensions.

If $\alpha > 0$, $A \geq \alpha > 0$, then A has a Krein extension distinct from the A_F, so there are multiple non-negative self-adjoint extensions.

Suppose $\alpha = 0$ and that B is some non-negative self-adjoint extension. Since A_F is the largest such extension, $0 \leq B \leq A_F$, so

$$(A_F + 1)^{-1} \leq (B+1)^{-1} \leq 1. \tag{3.1}$$

Since $\alpha = 0$, $\|(A_F + 1)^{-1}\| = 1$, so (3.1) implies that $\|(B+1)^{-1}\| = 1$. Since B has discrete spectrum by Theorem 5, this means 0 is an eigenvalue of B. But, by Theorem 5 again, A_F is the unique self-adjoint spectrum with a zero eigenvalue. Thus, $B = A_F$, that is, there is a unique non-negative self-adjoint extension. $\square$

Theorem 3.2 (last quarter of Theorem 2). *Suppose that A is a Jacobi matrix on the vectors of finite support and that A is non-negative. If A has a unique non-negative self-adjoint extension, then the associated Stieltjes moment problem is determinate.*

Proof. Clearly, if A is essentially self-adjoint, then the Hamburger problem is determinate and so, a fortiori, the Stieltjes problem is determinate. Thus, we need only consider the case where A has multiple self-adjoint extensions, but only one that is non-negative.

Then A has deficiency indices $(1,1)$. By Proposition 3.1, $\alpha = \inf \operatorname{spec}(A_F) = 0$. Moreover, by Theorem 5, 0 is a pure point of μ_F. Let $\varphi = P_{\{0\}}(A_F)\delta_0$. By Lemma 2.8, $\varphi \neq 0$. Then there exists $\varphi_n \in D(A)$ so $\varphi_n \to \varphi$ with $\|\varphi_n\| = \|\varphi\|$ and $(\varphi_n, A_F\varphi_n) \to (A_F\varphi, \varphi) = 0$. If $\mu_F(\{0\}) = \tau$, then $\|\varphi\|^2 = \langle \varphi, \delta_0\rangle = \tau$ so $\|\varphi_n\| = \sqrt{\tau}$ and $\langle \varphi_n, \delta_0\rangle \to \tau$.

Suppose ρ is some solution of the Stieltjes moment problem. Since $\varphi_n \to \varphi$ in $L^2(d\mu_F)$, φ_n is Cauchy in $L^2(d\rho)$, and so $\varphi_n \to f$ in $L^2(d\rho)$ and $\|f\| = \sqrt{\tau}$. Since $\int x\varphi_n(x)^2\, d\rho \to 0$, we conclude that $\int xf^2\, d\rho = 0$. Since ρ is a measure supported on $[0,\infty)$, we conclude $f(x) = 0$ for $x \neq 0$, and thus ρ has a pure point at zero also. Since $(\varphi_n, \delta_0) \to \tau$, we see that $\int f\, d\rho = \lim \int \varphi_n(x)\, d\rho(x) = \lim(\varphi_n, \delta_0) = \tau$. But $\int f^2\, d\rho = \|f\|^2 = \tau$ and $\int f\, d\rho = \tau$. Thus $f(0) = 1$ and so $\rho(\{0\}) = \tau$. But Theorem 5 asserts that any solution of the Hamburger problem distinct from μ_F has $\mu_F(\{0\}) < \tau$. We conclude that $\rho = \mu_F$, that is, that the solution of the Stieltjes problem is unique. $\square$

We will call the solution of the Stieltjes problem associated to the Friedrichs extension of A the *Friedrichs solution*. If the Stieltjes problem is indeterminate, then $A \geq \alpha > 0$ by Proposition 3.1 and Theorem 3.2. Moreover, since the Hamburger problem is indeterminate, $N = \ker(A) = \operatorname{span}[\pi(0)]$ has dimension 1, so the Krein extension exists and is distinct from the Friedrichs extension. We will call its spectral measure the *Krein solution* of the Stieltjes problem.

As discussed in the introduction, every indeterminate Stieltjes problem has associated to it an example of a determinate Stieltjes problem where the associated Hamburger problem is indeterminate. For by Proposition 3.1 and Theorem 3.2, the indeterminate Stieltjes problem is associated to an A where the bottom of the spectrum of A_F is some $f_0 > 0$. The moment problem $\{\gamma_m(-f_0)\}$ with $\gamma_m(-f_0) = \sum_{j=0}^m \binom{m}{j}\gamma_j(-f_0)^{m-j}$ will be determinate Stieltjes (since the associated A_F is the old $A_F - f_0$) but indeterminate Hamburger.

We summarize with

Theorem 3.3. *Suppose that $\{\gamma_n\}_{n=0}^\infty$ is a set of Stieltjes moments. Then, if γ is Hamburger indeterminate, there is a unique $c_0 \leq 0$ so that $\gamma(c_0)$ is Stieltjes determinate. Moreover, $\gamma(c)$ is Stieltjes indeterminate if $c > c_0$ and $\gamma(c)$ are not Stieltjes moments if $c < c_0$. In particular, if $\gamma(c)$ is Stieltjes determinate for two values of c, then γ is Hamburger determinate.*

Corollary 3.4. *If $\{\gamma_n\}_{n=0}^\infty$ is a set of Stieltjes moments and obeys*

$$|\gamma_n| \leq CR^n(2n)! \tag{3.2}$$

then $\{\gamma_n\}_{n=0}^\infty$ is Hamburger determinate.

Proof. By (3.2),

$$|\gamma_n(c)| \leq CR^n(2n)!\sum_{j=0}^n \binom{n}{j} c^j = C[R(c+1)]^n(2n)!$$

so by Proposition 1.5, $\{\gamma_n\}_{n=0}^\infty$ is Stieltjes determinate for all $c \geq 0$. By Theorem 3.3, it is Hamburger determinate.

§4. Transfer Matrices and the Indeterminate Moment Problem

In this section, we will analyze the indeterminate Hamburger problem in great detail, using the second-order difference equation associated to the Jacobi matrix A. In particular, we will prove Theorems 3, 4, and 5.

Throughout, we will fix a set of Hamburger moments $\{\gamma_m\}_{m=0}^\infty$. It will be convenient to define a linear functional $E(\,\cdot\,)$ on polynomials $P(X)$ by $E(X^m) \equiv \gamma_m$. Where we have polynomials P of several variables $X, Y, \dots$, we will indicate by $E_X(\,\cdot\,)$ the obvious map to polynomials of $Y, \dots$ with

$$E_X(X^m Y^{n_1} \dots) = \gamma_m Y^{n_1} \dots.$$

In (1.14), we defined the set of polynomials $P_n(X)$ by the three conditions, $\deg(P_n(X)) = n$, $E(P_n(X)P_m(X)) = \delta_{nm}$, and $P_n(X) = c_{nn}X^n + \cdots$ with $c_{nn} > 0$. We noted that with $\{a_n\}_{n=0}^\infty$, $\{b_n\}_{n=0}^\infty$, and $a_{-1} \equiv 1$, the elements of the Jacobi matrix associated to γ, the sequence $u_n = P_n(z)$; $n = 0, 1, 2, \dots$ obeys

$$a_n u_{n+1} + (b_n - z)u_n + a_{n-1}u_{n-1} = 0 \tag{4.1}$$

with

$$u_{-1} = 0, \qquad u_0 = 1. \tag{4.2}$$

We also introduced the sequence of polynomials $Q_n(X)$ of degree $n-1$ by requiring that $u_n = Q_n(z)$ solve (4.1) with the initial conditions

$$u_{-1} = -1, \qquad u_0 = 0. \tag{4.3}$$

Notice that the Wronskian $W(Q_{\cdot}(z), P_{\cdot}(z))(-1) = a_{-1}[Q_0(z)P_{-1}(z) - Q_{-1}(z)P_0(z)] = 1$. Thus, by (2.11) we have:

Proposition 4.1.

$$a_{k-1}[Q_k(z)P_{k-1}(z) - Q_{k-1}(z)P_k(z)] \equiv 1$$

The following is a useful formula for the Q's in terms of the P's. Note that since $\frac{X^n - Y^n}{(X-Y)} = \sum_{j=0}^{n-1} X^j Y^{n-1-j}$ for any polynomial P, $\frac{P(X)-P(Y)}{X-Y}$ is a polynomial in X and Y.

Theorem 4.2. *For $n \geq 0$,*

$$E_X\left(\frac{P_n(X) - P_n(Y)}{X - Y}\right) = Q_n(Y).$$

Proof. $\frac{[P_n(X)-P_n(Y)]}{(X-Y)}$ is a polynomial in X and Y of degree $n-1$, so we can define polynomials

$$R_n(Y) \equiv E_X\biggl(\frac{P_n(X)-P_n(Y)}{X-Y}\biggr).$$

Subtract the equations,

$$a_nP_{n+1}(X)+b_nP_n(X)+a_{n-1}P_{n-1}(X)=XP_n(X)$$
$$a_nP_{n+1}(Y)+b_nP_n(Y)+a_{n-1}P_{n-1}(Y)=YP_n(Y)$$

and see that for $n=0,1,2,\dots$ with $R_{-1}(Y)\equiv 0$:

$$\begin{aligned}a_nR_{n+1}(Y)+b_nR_n(Y)+a_{n-1}R_{n-1}(Y)&=E_X\biggl(\frac{XP_n(X)-YP_n(Y)}{X-Y}\biggr)\\&=E_X\biggl(\frac{YP_n(X)-YP_n(Y)}{X-Y}+P_n(X)\biggr)\\&=YR_n(Y)+\delta_{n0}.\end{aligned}$$

Replace the abstract variable Y with a complex variable z and let $\tilde R_n(z)=R_n(z)$ if $n\geq 0$ but $\tilde R_{-1}(z)=-1$. Then

$$a_n\tilde R_{n+1}(z)+b_n\tilde R_n(z)+a_{n-1}\tilde R_{n-1}(z)=z\tilde R_n(z)$$

(since the δ_{n0} term becomes $-a_{n-1}\tilde R_{n-1}(z)$ for $n=0$). Moreover,

$$\tilde R_{-1}(z)=-1,\qquad \tilde R_0(z)=E_X\biggl(\frac{1-1}{X-Y}\biggr)=0$$

so by uniqueness of solutions of (4.1) with prescribed initial conditions, $\tilde R_n(z)=Q_n(z)$, that is, for $n\geq 0$, $R_n=Q_n$, as claimed. $\square$

One consequence of Theorem 4.2 is that $P_n(X)$ and $Q_n(X)$ have the same leading coefficient, that is, if $P_n(X)=c_{nn}X^n+\cdots$, then $Q_n(X)=c_{nn}X^{n-1}+\cdots$.

The following calculation is part of the standard theory [1] and plays a critical role in what follows:

Theorem 4.3. *Let ρ solve the moment problem and assume $z\in\mathbb{C}\backslash\mathbb{R}$. Set $\zeta=G_\rho(z)\equiv\int\frac{d\rho(x)}{x-z}$. Then*

$$\langle (x-z)^{-1},P_n(x)\rangle_{L^2(d\rho)}=Q_n(z)+\zeta P_n(z). \tag{4.4}$$

In particular,

$$\sum_{n=0}^\infty |Q_n(z)+\zeta P_n(z)|^2\leq\frac{\operatorname{Im}\zeta}{\operatorname{Im} z} \tag{4.5}$$

with equality if ρ is a von Neumann solution.

Remark. We will eventually see (Proposition 4.15 and its proof) that the "if" in the last sentence can be replaced by "if and only if."

Proof.

$$\int \frac{P_n(x)}{x-z}\,d\rho(x) = \zeta P_n(z) + \int \frac{P_n(x)-P_n(z)}{x-z}\,d\rho(x) = \zeta P_n(z) + Q_n(z)$$

by Theorem 4.2. This is just (4.4). (4.5) is just Parseval's inequality for the orthonormal set $\{P_n(x)\}_{n=0}^\infty$ in $L^2(d\rho)$ if we note that

$$\int \frac{d\rho(x)}{|x-z|^2} = \frac{1}{z-\bar z}\int d\rho(x)\left[\frac{1}{x-z} - \frac{1}{\bar x - \bar z}\right] = \frac{\operatorname{Im}\zeta}{\operatorname{Im} z}\,.$$

If ρ comes from a self-adjoint extension, by construction of $\mathcal{H}^{(\gamma)}$, $\{P_n(x)\}_{n=0}^\infty$ is an orthonormal basis for $L^2(d\rho)$, so equality holds in (4.5). $\square$

Remark. In $\mathcal{H}^{(\gamma)}$, thought of as limits of polynomials, the vector with components $Q_n(z)+\zeta P_n(z)$ is represented by

$$\sum_n [Q_n(z) + \zeta P_n(z)] P_n(X).$$

This product of P's may seem strange until one realizes that $\sum_{n=1}^N P_n(y)P_n(x)$ is a reproducing kernel in $L^2(d\rho)$ for polynomials of degree N. This links the construction to ideas in Landau [19].

Given Theorem 2, the following proves the equivalence of parts (i), (ii), (iii), and (vii) for $z \in \mathbb{C}\backslash\mathbb{R}$ of Theorem 3.

Proposition 4.4. *Suppose that $z_0 \in \mathbb{C}\backslash\mathbb{R}$. Then the following are equivalent:*

(i) *The Jacobi matrix A is not essentially self-adjoint.*
(ii) $\pi(z_0) = \{P_n(z_0)\}_{n=0}^\infty$ *is in* ℓ^2.
(iii) $\xi(z_0) = \{Q_n(z_0)\}_{n=0}^\infty$ *is in* ℓ^2.
(iv) *Both* $\pi(z_0)$ *and* $\xi(z_0)$ *are in* ℓ^2.

Moreover, when any of these conditions holds, there is a closed disk of positive radius, $\mathcal{D}(z_0)$, in the same half-plane as z_0 so that for any solution ρ of the moment problem, $\zeta = G_\rho(z_0) \in \mathcal{D}(z_0)$. The values of ζ when ρ is a von Neumann solution lie on $\partial\mathcal{D}(z_0)$ and fill this entire boundary. Every point in $\mathcal{D}(z_0)$ is the value of $G_\rho(z_0)$ for some ρ solving the moment problem.

In addition, if these conditions hold, $\pi(z_0)$ and $\xi(z_0)$ lie in $D(A^*)\backslash D(A)$.

Remarks. 1. One can show (using (2.11)) that the center of the disk is

$$\lim_{n\to\infty} -\frac{Q_n(z_0)\,\overline{P_{n-1}(z_0)} - Q_{n-1}(z_0)\,\overline{P_n(z_0)}}{P_n(z_0)\overline{P_{n-1}(z_0)} - P_{n-1}(z_0)\,\overline{P_n(z_0)}}$$

and the radius is

$$\frac{1}{2|\mathrm{Im}\, z_0|}\ \frac{1}{\|\pi(z_0)\|^2} \tag{4.6}$$

but these explicit formulae will play no role in our discussions.

2. We will see later (Theorem 4.14) that if ρ is not a von Neumann solution, then $\zeta \in \mathcal{D}(z_0)^{\mathrm{int}}$.

Proof. Since A is real, A fails to be essentially self-adjoint if and only if there is a non-zero solution of $(A^* - z_0)u = 0$. By Theorem 2.6 and the unique solubility of second-order difference operators given $u_{-1} = 0$ and u_0, every such solution has $u_n = u_0 P_n(z_0)$ so (i) is equivalent to (ii). Let $\zeta = G_\rho(z_0)$ for some von Neumann solution. Then $\xi(z_0) + \zeta\pi(z_0) \in \ell^2$, so (ii) is equivalent to (iii) or (iv).

If (i)–(iv) hold, then (4.5) has the form

$$a|\zeta|^2 + b\zeta + \bar{b}\bar{\zeta} + c \le 0,$$

where $a = \|\pi(z_0)\|^2$, $c = \|\xi(z_0)\|^2$, and $b = 2\langle \xi(z_0), \pi(z_0)\rangle - \frac{i}{2\,\mathrm{Im}\, z_0}$. The set where this inequality holds is always a disk, $\mathcal{D}(z_0)$, although a priori, it could be empty depending on the values of a, b, c. However, by Theorem 2.11, we know that there are multiple ζ's obeying (4.5) so the disk must have strictly positive radius. By Theorem 4.3, ζ's for von Neumann solutions obey equality in (4.5) and so lie in $\partial\mathcal{D}(z_0)$.

The self-adjoint extensions are parametrized by a circle (unitaries from $\mathcal{K}_+$ to $\mathcal{K}_-$) in such a way that the map from the parametrization to values of $(\delta_0, (B_t - z_0)^{-1}\delta_0)$ is continuous. By Theorem 2.11, this map is one-one. Every one-one continuous map of the circle to itself is surjective, so all of $\partial\mathcal{D}(z_0)$ occurs.

Given a point ζ in $\mathcal{D}(z_0)^{\mathrm{int}}$, find ζ_0 and ζ_1 in $\partial\mathcal{D}(z_0)$ and $\theta \in (0,1)$ so $\zeta = \theta\zeta_0 + (1-\theta)\zeta_1$. If μ_0, μ_1 are the von Neumann solutions that have $G_{\mu_i}(z_0) = \zeta_i$ $(i = 0, 1)$, then $\rho = \theta\mu_0 + (1-\theta)\mu_1$ is a measure solving the moment problem with $G_\rho(z_0) = \zeta$.

If (iv) holds, then $\pi(\bar{z}_0), \xi(z_0) \in D(A^*)$. By (2.14) and Proposition 1.4, $\langle A^*\pi(\bar{z}_0), \xi(z_0)\rangle - \langle \pi(\bar{z}_0), A^*\xi(z_0)\rangle = -1$, so neither $\pi(\bar{z}_0)$ nor $\xi(z_0)$ lies in $D(A)$. $\square$

Remark. The Cayley transform way of looking at self-adjoint extensions says that for any $z_0 \in \mathbb{C}\backslash\mathbb{R}$,

$$(B_t - \bar{z}_0)(B_t - z_0)^{-1} = V(z_0) + e^{i\theta(z_0,t)}X(z_0),$$

where $V(z_0)$ is the t-independent map $(\bar{A} - \bar{z}_0)(\bar{A} - z_0)^{-1}$ from $\overline{\mathrm{Ran}(A - z_0)}$ to $\overline{\mathrm{Ran}(A - \bar{z}_0)}$ and $X(z_0)$ is any isometry from $\ker(A^* - \bar{z}_0)$ to $\ker(A^* - z_0)$ extended to $\mathcal{H}$ as a partial isometry. θ is a parametrization depending on z_0, t (and the choice of $X(z_0)$), but the theory guarantees that as t varies through all possible values, $e^{i\theta}$ runs through the full circle in an injective manner. Now $(B_t - \bar{z}_0)(B_t - z_0)^{-1} = 1 + 2i(\mathrm{Im}\, z_0)(B_t - z_0)^{-1}$, so

$$(\delta_0, (B_t - z_0)^{-1}\delta_0) = [2i(\mathrm{Im}\, z_0)]^{-1}[-1 + (\delta_0, V(z_0)\delta_0) + e^{i\theta(z_0,t)}(\delta_0, X(z_0)\delta_0)]$$

is seen directly to be a circle. Since one can take $X(z_0)$ to be

$$(\delta_n, X(z_0)\delta_m) = \frac{P_m(\bar{z}_0)P_n(z_0)}{\sum_{j=0}^\infty |P_j(z_0)|^2}$$

and $P_0(z) \equiv 1$, we even see that the radius of the circle is given by (4.6).

Corollary 4.5. *If a Hamburger problem is indeterminate, then* $\sum_{n=0}^{\infty} |a_n|^{-1} < \infty$. *In particular, if* $\sum_{n=0}^{\infty} |a_n|^{-1} = \infty$, *(e.g.,* $a_n \equiv 1$*), then the Hamburger problem is determinate. If*

$$\sum_{n=1}^{\infty} \gamma_{2n}^{-1/2n} = \infty,$$

then the Hamburger problem is determinate. If

$$\sum_{n=1}^{\infty} \gamma_n^{-1/2n} = \infty$$

for a set of Stieltjes moments, that problem is both Stieltjes and Hamburger determinate.

Remarks. 1. The last pair of assertions is called Carleman's criterion. It generalizes Proposition 1.5 and proves uniqueness in some cases where growth doesn't imply analyticity of the Fourier transform.

2. See Corollary 5.24 for the Stieltjes analog of the first assertion.

Proof. By Proposition 4.1 and the Schwarz inequality,

$$\sum_{n=0}^{N} |a_n|^{-1} \leq 2\biggl(\sum_{n=0}^{N+1} |P_n(z)|^2\biggr)^{1/2} \biggl(\sum_{n=0}^{N+1} |Q_n(z)|^2\biggr)^{1/2}.$$

Thus, divergence of $\sum_{n=0}^{\infty} |a_n|^{-1}$ implies that either π or ξ (or both) fail to be ℓ_2, and so determinacy.

Consider Carleman's criterion in the Hamburger case. By induction in n and (4.1) starting with $P_0(x) = 1$, we see that

$$P_n(x) = (a_1 \dots a_n)^{-1} x^n + \text{lower order},$$

so $\langle (a_1 \dots a_n)^{-1} x^n, P_n(x) \rangle = 1$ and thus, by the Schwartz inequality,

$$1 \leq \gamma_{2n} (a_1 \dots a_n)^{-2}$$

hence

$$\gamma_{2n}^{-1/2n} \leq (a_1 \dots a_n)^{-1/n}.$$

Therefore our result follows from the divergence criteria proven at the start of the proof and the inequality

$$\sum_{j=1}^{n} (a_1 \dots a_j)^{-1/j} \leq 2e \sum_{j=1}^{n} a_j^{-1}$$

(which is actually known to hold with e in place of $2e$).

To prove this, note first that $1+x \leq e^x$ so $(1+n^{-1})^n \leq e$ so using induction, $n^n \leq e^n n!$, so by the geometric-arithmetic mean inequality,

$$\begin{aligned}(a_1 \dots a_j)^{-1/j} &= (a_1^{-1} 2a_2^{-1} \dots j a_j^{-1})^{1/j} (j!)^{-1/j} \\ &\leq \frac{e}{j^2} \sum_{k=1}^{j} k a_k^{-1}.\end{aligned}$$

Thus,

$$\sum_{j=1}^{n} (a_1 \dots a_j)^{-1/j} \leq e \sum_{k=1}^{n} a_k^{-1} \left(\sum_{j=k}^{n} \frac{k}{j^2} \right) \leq 2e \sum_{j=1}^{n} a_j^{-1}$$

since

$$\sum_{j=k}^{\infty} \frac{k}{j^2} \leq \frac{1}{k} + k \int_k^{\infty} \frac{dy}{y^2} \leq 2.$$

By Proposition 1.6, Carleman's criterion in the Hamburger case means that if a set of Stieltjes moments obeys $\sum_{n=1}^{\infty} (\gamma_n)^{-1/2n} = \infty$, then it is Stieltjes determinate. Thus by Theorem 3.3, it suffices to show that

$$\sum_{n=1}^{\infty} (\gamma_n(c))^{-1/2n} \geq D(c) \sum_{n=1}^{\infty} \gamma_n^{-1/2n}$$

for $c > 0$ and $D(c) < \infty$ to conclude Hamburger determinacy.

Note first that $\frac{\gamma_{j+1}}{\gamma_j} \geq \frac{\gamma_j}{\gamma_{j-1}}$ by the Schwarz inequality. Thus, if $\alpha = \frac{\gamma_0}{\gamma_1}$, we have that

$$\gamma_{n-j} \leq \gamma_n \alpha^j.$$

Therefore,

$$\gamma_n(c) \leq \gamma_n \sum_{j=0}^{n} \binom{n}{j} c^j \alpha^j = (1 + c\alpha)^n \gamma_n$$

and so

$$\sum_{n=1}^{\infty} (\gamma_n(c))^{-1/2n} \geq (1 + c\alpha)^{-1/2} \sum_{n=1}^{\infty} \gamma_n^{-1/2n}. \quad \square$$

To complete the proof of Theorem 3, we need to show that if every solution of $[(A^* - z_0)u]_n = 0$ $(n \geq 1)$ is ℓ^2 for a fixed $z = z_0$, the same is true for all $z \in \mathbb{C}$ and that $\frac{\partial \pi}{\partial x}$, $\frac{\partial \xi}{\partial x}$ are in ℓ^2. We will do this by the standard method of variation of parameters. So we write a general solution of $[(A^* - z)u]_n = 0$ $(n \geq 1)$ in terms of $P_n(z_0)$ and $Q_n(z_0)$ using

$$\begin{pmatrix} u_{n+1} \\ u_n \end{pmatrix} \equiv \alpha_n \begin{pmatrix} P_{n+1}(z_0) \\ P_n(z_0) \end{pmatrix} + \beta_n \begin{pmatrix} Q_{n+1}(z_0) \\ Q_n(z_0) \end{pmatrix}. \tag{4.7}$$

Since $W(P.(z_0), Q.(z_0)) = -1$, the two vectors on the right of (4.7) are linearly independent, and so they span $\mathbb{C}^2$ and (α_n, β_n) exist and are unique. Indeed, by the Wronskian relation:

$$\alpha_n = W(Q.(z_0), u)(n) \tag{4.8a}$$

$$\beta_n = -W(P.(z_0), u)(n). \tag{4.8b}$$

A straightforward calculation using the fact that P, Q obey (4.1) with $z = z_0$, (2.11), and (4.8) shows that (4.1) at n is equivalent to

$$\begin{pmatrix} \alpha_n \\ \beta_n \end{pmatrix} = [1 + (z - z_0) S(n, z_0)] \begin{pmatrix} \alpha_{n-1} \\ \beta_{n-1} \end{pmatrix}, \tag{4.9}$$

where

$$S(n, z_0) = \begin{pmatrix} -Q_n(z_0)P_n(z_0) & -Q_n(z_0)Q_n(z_0) \\ P_n(z_0)P_n(z_0) & P_n(z_0)Q_n(z_0) \end{pmatrix}. \tag{4.10}$$

For example, using (2.11) and (4.7) for $n \to n-1$:

$$\begin{aligned} \alpha_n &= W(Q.(z_0), u)(n) \\ &= W(Q.(z_0), u)(n-1) + (z_0 - z) Q_n(z_0) u_n \\ &= \alpha_{n-1} - (z - z_0) Q_n(z_0) \{\alpha_{n-1} P_n(z_0) + \beta_{n-1} Q_n(z_0)\}. \end{aligned}$$

Notice that

$$S^2 = \det(S) = \operatorname{Tr}(S) = 0. \tag{4.11}$$

The following is obvious and explains why ℓ^2 solutions are so natural:

If $\pi(z_0) = \{P_n(z_0)\}_{n=0}^\infty$ and $\xi(z_0) = \{Q_n(z_0)\}_{n=0}^\infty$ are *both* in ℓ^2, then

$$\sum_{n=0}^\infty \|S(n, z_0)\| < \infty. \tag{4.12}$$

Lemma 4.6. *Let A_n be a sequence of matrices with $\sum_{n=0}^\infty \|A_n\| < \infty$. Let $D_N(z) = (1 + zA_N)(1 + zA_{N-1}) \dots (1 + zA_0)$. Then $D_\infty(z) = \lim D_N(z)$ exists for each $z \in \mathbb{C}$ and defines an entire function of z obeying*

$$\|D_\infty(z)\| \le c_\varepsilon \exp(\varepsilon |z|)$$

for each $\varepsilon > 0$.

Proof. Notice first that

$$\|(1 + B_N) \dots (1 + B_0)\| \le \prod_{j=0}^N (1 + \|B_j\|) \le \exp\biggl(\sum_{j=0}^N \|B_j\|\biggr) \tag{4.13}$$

and that

$$\|(1+B_N)\dots(1+B_0)-1\| \le \prod_{j=0}^{N}(1+\|B_j\|)-1 \le \exp\biggl(\sum_{j=0}^{N}\|B_j\|\biggr)-1. \tag{4.14}$$

From (4.14), we see that

$$\begin{aligned}\|D_{N+j}(z)-D_N(z)\| &\le \biggl[\exp\biggl(|z|\sum_{N+1}^{N+j}\|A_j\|\biggr)-1\biggr]\|D_N(z)\| \\ &\le \biggl[\exp\biggl(|z|\sum_{N+1}^{\infty}\|A_j\|\biggr)-1\biggr]\exp\biggl(|z|\sum_{j=0}^{N}\|A_j\|\biggr),\end{aligned}$$

from which it follows that $D_N(z)$ is Cauchy uniformly for z in balls of $\mathbb{C}$. Thus, D_∞ exists and is entire in z. By (4.13),

$$\|D_\infty(z)\| \le \prod_{j=0}^{N}(1+|z|\|A_j\|)\exp\biggl(|z|\sum_{j=N+1}^{\infty}\|A_j\|\biggr),$$

so given ε, choose N so $\sum_{j=N+1}^{\infty}\|A_j\| \le \frac{\varepsilon}{2}$ and use the fact that the polymonial $\prod_{j=0}^{N}(1+|z|\|A_j\|)$ can be bounded by $c_\varepsilon\exp(\frac{1}{2}\varepsilon|z|)$. $\square$

Given Proposition 4.4 and Theorem 2.14, the following completes the proof of Theorem 3:

Theorem 4.7. *Let A be a Jacobi matrix and consider solutions of (4.1) for $z\in\mathbb{C}$. If for some $z_0\in\mathbb{C}$, all solutions are in ℓ^2, then that is true for each $z\in\mathbb{C}$. Moreover, $\pi(z)$ and $\xi(z)$ are analytic ℓ_2-valued functions so, in particular, $\frac{\partial\pi}{\partial z},\frac{\partial\xi}{\partial z}\in\ell_2$ for all z. The disk $\mathcal{D}(z_0)$ varies continuously as z runs through $\mathbb{C}_+$.*

Proof. Define

$$T(n,-1;z,z_0)=(1+(z-z_0)S(n,z_0))\dots(1+(z-z_0)S(0,z_0)).$$

By (4.12) and Lemma 4.6,

$$\sup_n\|T(n,-1,;z,z_0)\| \le \exp\biggl(|z-z_0|\sum_{j=0}^{\infty}\|S(j,z)\|\biggr)<\infty.$$

Thus for any initial $\binom{\alpha_{-1}}{\beta_{-1}}$, if u has the form (4.7), then $\sup_n\|\binom{\alpha_n}{\beta_n}\| \le \sup_n\|T(n,-1;z,z_0)\|\|\binom{\alpha_{-1}}{\beta_{-1}}\| \equiv C$. Thus, $u_n=\alpha_nP_n(z_0)+\beta_nQ_n(z_0)$ has $|u_n|^2\le C^2[P_n(z_0)^2+Q_n(z_0)^2]$ which is in ℓ_1. Since $\pi(z)$ is associated to $T(n,-1;z,z_0)\binom{1}{0}$ and $\xi(z)$

is associated to $T(n,-1;z,z_0)\binom{0}{1}$, the claimed analyticity holds because $\sup_n \|T(n,-1;z,z_0)\|$ is bounded as z varies in bounded sets.

Continuity of $\mathcal{D}(z_0)$ follows from the formula for $\partial\mathcal{D}(z_0)$, viz. $w \in \partial\mathcal{D}(z_0)$ if and only if

$$\|\pi(z_0)\|^2|w|^2 + 2\operatorname{Re}\biggl[\biggl(2\langle\xi(z_0),\pi(z_0)\rangle - \frac{i}{2\operatorname{Im} z_0}\biggr)w\biggr] + \|\xi(z_0)\|^2 = 0. \quad \square$$

By Theorem 3 and Lemma 4.6, if the Hamburger problem is indeterminate,

$$T(\infty,-1;z,z_0) \equiv \lim_{n\to\infty} T(n,-1;z,z_0) \tag{4.15}$$

exists. We define four functions $A(z)$, $B(z)$, $C(z)$, $D(z)$ by

$$T(\infty,-1;z,z_0=0) = \begin{pmatrix} -B(z) & -A(z) \\ D(z) & C(z) \end{pmatrix}. \tag{4.16}$$

The *Nevanlinna matrix* is defined by

$$N(z) = \begin{pmatrix} A(z) & C(z) \\ B(z) & D(z) \end{pmatrix}. \tag{4.17}$$

Theorem 4.8.

(i) *Each of the functions A, B, C, D is an entire function obeying*

$$|f(z)| \le c_\varepsilon \exp(\varepsilon|z|)$$

for each $\varepsilon > 0$.

(ii) *For z small,*

$$B(z) = -1 + O(z) \tag{4.18a}$$

and

$$D(z) = \alpha z + O(z^2) \tag{4.18b}$$

with $\alpha > 0$.

(iii) *$AD - BC \equiv 1$.*

Proof. (i) follows from Lemma 4.6. (ii) follows if we note that

$$T(\infty,-1;z,z_0=0) = 1 + z\sum_{n=0}^{\infty} S(n,z_0=0) + O(z^2).$$

(4.18a) is immediate and (4.18b) follows since (4.10) says that $\alpha = \sum_{n=0}^{\infty} P_n(0)^2 > 0$. (iii) holds since by (4.11), $\det T = 1$. $\square$

For our purposes, the formula for A, B, C, D as matrix elements of an infinite product is sufficient, but there is an infinite sum formula connected to standard equations for perturbed solutions (see, e.g., [32, 11]) that lets us make contact with the more usual definitions [1].

Theorem 4.9. *If the Hamburger problem is indeterminate, then,*

$$A(z) = z \sum_{n=0}^{\infty} Q_n(0)Q_n(z)$$

$$B(z) = -1 + z \sum_{n=0}^{\infty} Q_n(0)P_n(z)$$

$$C(z) = 1 + z \sum_{n=0}^{\infty} P_n(0)Q_n(z)$$

$$D(z) = z \sum_{n=0}^{\infty} P_n(0)P_n(z).$$

Proof.

$$\begin{aligned} T(n,-1;z,z_0=0) &= (1+zS(n,z_0=0))\dots(1+zS(0,z_0=0)) \\ &= 1 + \sum_{j=0}^{n} zS(j,z_0=0) \prod_{k=0}^{j-1} (1+zS(k,z_0=0)) \end{aligned}$$

so it suffices to show that

$$\begin{aligned} &S(j,z_0=0)(1+zS(j-1,z_0=0))\dots(1+zS(0,z_0=0)) \\ &\qquad = \begin{pmatrix} -Q_j(0)P_j(z) & -Q_j(0)Q_j(z) \\ P_j(0)P_j(z) & P_j(0)Q_j(z) \end{pmatrix}. \end{aligned} \tag{4.19}$$

By definition,

$$(1+zS(j-1,z_0=0))\dots(1+zS(0,z_0=0)) = \begin{pmatrix} \alpha_{j-1}^{(1)} & \alpha_{j-1}^{(2)} \\ \beta_{j-1}^{(1)} & \beta_{j-1}^{(2)} \end{pmatrix},$$

where

$$\alpha_{j-1}^{(1)} \begin{pmatrix} P_j(0) \\ P_{j-1}(0) \end{pmatrix} + \beta_{j-1}^{(1)} \begin{pmatrix} Q_j(0) \\ Q_{j-1}(0) \end{pmatrix} = \begin{pmatrix} P_j(z) \\ P_{j-1}(z) \end{pmatrix}$$

and

$$\alpha_{j-1}^{(2)} \begin{pmatrix} P_j(0) \\ P_{j-1}(0) \end{pmatrix} + \beta_{j-1}^{(2)} \begin{pmatrix} Q_j(0) \\ Q_{j-1}(0) \end{pmatrix} = \begin{pmatrix} Q_j(z) \\ Q_{j-1}(z) \end{pmatrix}.$$

Thus by (4.10),

$$\begin{aligned} \text{LHS of (4.19)} &= \begin{pmatrix} -Q_j(0)[\alpha_{j-1}^{(1)}P_j(0) + \beta_{j-1}^{(1)}Q_j(0)] & -Q_j(0)[\alpha_{j-1}^{(2)}P_j(0) + \beta_{j-1}^{(2)}Q_j(0)] \\ P_j(0)[\alpha_{j-1}^{(1)}P_j(0) + \beta_{j-1}^{(1)}Q_j(0)] & P_j(0)[\alpha_{j-1}^{(2)}P_j(0) + \beta_{j-1}^{(2)}Q_j(0)] \end{pmatrix} \\ &= \text{RHS of (4.19)}. \qquad \square \end{aligned}$$

$\pi(0) = \{P_n(0)\}$ and $\xi(0) = \{Q_n(0)\}$ span $D(A^*)/D(A)$ by Proposition 4.4. Notice that $A^*\pi(0) = 0$ while $A^*\xi(0) = \delta_0$, so $\langle \pi(0), A^*\xi(0)\rangle = 1$ and (2.7) holds. Thus, we can parametrize the self-adjoint extensions B_t of A by

$$D(B_t) = D(A) + \{\alpha(t\pi(0) + \xi(0)) \mid \alpha \in \mathbb{C}\} \tag{4.20a}$$

if $t < \infty$ and

$$D(B_\infty) = D(A) + \{\alpha\pi(0)\}. \tag{4.20b}$$

This is equivalent to defining t by

$$t = (\delta_0, B_t^{-1}\delta_0). \tag{4.20c}$$

Theorem 4.10. *For each $t \in \mathbb{R} \cup \{\infty\}$ and $z \in \mathbb{C}\backslash\mathbb{R}$,*

$$(\delta_0, (B_t - z)^{-1}\delta_0) = -\frac{C(z)t + A(z)}{D(z)t + B(z)}\,. \tag{4.21}$$

Proof. Let us sketch the proof before giving details:

$$T(-1, \infty; z, z_0 = 0) \equiv T(\infty, -1; z, z_0 = 0)^{-1}. \tag{4.22}$$

Then

$$\begin{pmatrix} \alpha_{-1} \\ \beta_{-1} \end{pmatrix} \equiv T(-1, \infty; z, z_0 = 0)\begin{pmatrix} t \\ 1 \end{pmatrix} \tag{4.23}$$

is such that the u_n associated to $\binom{\alpha_{-1}}{\beta_{-1}}$ obeys (4.1) and is asymptotically $t\pi(0)+\xi(0)$ and so in $D(B_t)$. $(B_t - z)^{-1}\delta_0$ will thus be $-\frac{u_t}{u_t(-1)}$ and $(\delta_0, (B_t - z)^{-1}\delta_0)$ will be $-\frac{u_t(0)}{u_t(-1)}$. But $u_t(0) = \alpha_{-1}$ and $u_t(-1) = -\beta_{-1}$ so $(\delta_0, B_t - z)^{-1}\delta_0)$ will be $\frac{\alpha_{-1}}{\beta_{-1}}$, which is given by (4.21).

Here are the details. If $\varphi \in D(A^*)$, then by (2.14), $\varphi \in D(B_t)$ if and only if

$$\lim_{n\to\infty} W(\varphi, t\pi(0) + \xi(0))(n) = 0. \tag{4.24}$$

Suppose u solves (4.1) for a given z. Then $u \in D(A^*)$ and u has the form (4.7), where by (4.15), $\lim_{n\to\infty} \binom{\alpha_n}{\beta_n} = \binom{\alpha_\infty}{\beta_\infty}$ exists. Clearly,

$$W(u, t\pi(0) + \xi(0))(n) = -\alpha_n + \beta_n t$$

so (4.24) holds if and only if

$$\alpha_\infty = t\beta_\infty.$$

Thus, if $T(-1, \infty; z, z_0 = 0)$ is given by (4.22), then $\binom{\alpha_{-1}}{\beta_{-1}}$ given by (4.23) is initial data for a solution u of (4.1) that has $u \in D(B_t)$. A solution u of (4.1) has

$$(A^* - z)u = -u_{-1}\delta_0$$

and thus, if u is associated to the data in (4.23),

$$(B_t - z)u = -u_{-1}\delta_0$$

and

$$(\delta_0, (B_t - z)^{-1}\delta_0) = -\frac{u_0}{u_{-1}}\,.$$

But

$$\begin{pmatrix} u_0 \\ u_{-1} \end{pmatrix} = \alpha_{-1}\begin{pmatrix} P_0(0) \\ P_{-1}(0) \end{pmatrix} + \beta_{-1}\begin{pmatrix} Q_0(0) \\ Q_{-1}(0) \end{pmatrix} = \begin{pmatrix} \alpha_{-1} \\ -\beta_{-1} \end{pmatrix}$$

so

$$(\delta_0, (B_t - z)^{-1}\delta_0) = \frac{\alpha_{-1}}{\beta_{-1}}\,.$$

Since $T(\infty, -1; z, z_0 = 0)$ has the form (4.16) and has determinant 1, its inverse has the form

$$\begin{pmatrix} C(z) & A(z) \\ -D(z) & -B(z) \end{pmatrix}$$

and so $\alpha_{-1} = C(z)t + A(z)$, $\beta_{-1} = -D(z)t - B(z)$. Thus (4.21) is proven. $\square$

Remark. Our convention for the parameter t differs from that in Akhiezer [1], which is the traditional one! If $s = -t^{-1}$, then

$$-\frac{Ct + A}{Dt + B} = -\frac{As - C}{Bs - D}\,.$$

The parameter s is what he calls t. Our $\Phi(z)$ later and his $\Phi(z)$, which I will call $\Psi(z)$, are related by $\Phi(z) = -\Psi(z)^{-1}$. Since this transformation takes Herglotz functions to themselves, we both deal with Herglotz functions. See [9] for an interesting alternate reparametrization.

We turn next to half of Theorem 5. We will prove that each B_t has point spectrum with any two disjoint. The condition that $\mu_t(\{t\}) > \rho(\{t\})$ for any other solution of the moment problem will wait until after we have proven Theorem 4.

Theorem 4.11 (half of Theorem 5). *Suppose the Hamburger problem is indeterminate. Each B_t has pure point spectrum only. The eigenvalues of the different B_t's are distinct and every $x \in \mathbb{R}$ is an eigenvalue of some B_t. If x is an eigenvalue of B_t, then*

$$\mu_t(\{x\}) = \frac{1}{\sum_{n=0}^{\infty} |P_n(x)|^2}\,. \tag{4.25}$$

Moreover, if $\lambda_n(B_t)$ are the eigenvalues of B_t (ordered in some convenient way), then for any $p > 1$,

$$\sum_n |\lambda_n(B_t)|^{-p} < \infty. \tag{4.26}$$

Proof. Let μ_t be the spectral measure for B_t. By Theorem 4.10,

$$\int \frac{d\mu_t(x)}{x-z} = -\frac{C(z)t + A(z)}{D(z)t + B(z)}$$

is a meromorphic function of z, since A, B, C, D are entire. That implies that μ_t is pure point only and these points are given by solutions of

$$D(z)t + B(z) = 0.$$

Since A, B, C, D are real when $z = x$ is real, for any x, $x \in \operatorname{spec}(B_t)$ for $t = -\frac{B(x)}{D(x)}$. Since $AD - BC \equiv 1$, B and D have no simultaneous zeros, so the eigenvalues are distinct for different t's. (4.26) is a standard result on the zeros of an entire function like $D(z)t+B(z)$, which obeys (i) of Theorem 4.8.

To prove (4.25), note that if x is an eigenvalue of B_t, then the corresponding normalized eigenvector φ obeys $A^*\varphi = x\varphi$. It follows that $\varphi_n = \varphi_0 P_n(x)$ and then by normalization, that $\varphi_0^2 = 1/\sum_{n=0}^{\infty} |P_n(x)|^2$. Thus, $\mu_t(\{x\}) = \varphi_0^2$ is given by (4.25). $\square$

Now define the map $F(z) : \mathbb{C} \cup \{\infty\} \to \mathbb{C} \cup \{\infty\}$ by

$$F(z)(w) = -\frac{C(z)w + A(z)}{D(z)w + B(z)}\,. \tag{4.27}$$

$F(z)$ as a fractional linear transformation is one-one and onto, and takes $\mathbb{R} \cup \{\infty\}$ onto a circle or straight line. By Proposition 4.4 and (4.21), $F(z)[\mathbb{R} \cup \{\infty\}]$ is precisely the circle $\partial\mathcal{D}(z)$ when $\operatorname{Im} z \neq 0$.

Proposition 4.12. *If* $\operatorname{Im} z > 0$, *$F(z)$ maps the upper half-plane* $\mathbb{C}_+ = \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}$ *onto the interior of the disk* $\mathcal{D}(z)^{\text{int}}$.

Proof. For each $z \in \mathbb{C}\backslash\mathbb{R}$, $F(z)$ must map $\mathbb{C}_+$ onto either $\mathcal{D}(z)^{\text{int}}$ or $\mathbb{C}\backslash\mathcal{D}(z)$ since $\mathbb{R}$ is mapped to $\partial\mathcal{D}(z)$ and a fractional linear transformation maps $\mathbb{C}\cup\{\infty\}$ to itself bijectively. Thus it suffices to show $F(z)[i] \in \mathcal{D}(z)^{\text{int}}$ for all z with $\operatorname{Im} z > 0$. But $F(z)[i]$ moves analytically, and so continuously. It can only move from $\mathcal{D}(z)^{\text{int}}$ to $\mathbb{C}\backslash\mathcal{D}(z)$ by lying on $\partial\mathcal{D}(z)$, which is impossible if $\operatorname{Im} z > 0$ since then $\partial\mathcal{D}(z) = F(z)[\mathbb{R} \cup \{\infty\}]$. Thus it suffices to show $F(z)[i] \in \mathcal{D}(z)^{\text{int}}$ for $z = ix$ with $x > 0$ and small.

Now, $F(z)[i] \in \mathcal{D}(z)^{\text{int}}$ if and only if $F(z)$ takes the lower half-plane to $\mathbb{C}\cup\{\infty\}\backslash\mathcal{D}(z)$, which holds if and only if $F(z)^{-1}[\infty]$ is in the lower half-plane. Thus it suffices to show for x small and positive that $F(ix)^{-1}[\infty] \in \mathbb{C}_-$.

$F(ix)^{-1}[\infty]$ is that w with $D(ix)w + B(ix) = 0$, that is, $w = -\frac{B(ix)}{D(ix)}$. But by (4.18), $B(ix) = -1 + O(x)$ and $D(ix) = i\alpha x + O(x^2)$ with $\alpha > 0$, so $w = -i\alpha^{-1}x^{-1} + O(1)$ lies in $\mathbb{C}_-$, which suffices to prove the proposition. $\square$

We now follow the classical argument of Nevanlinna [29] to obtain Theorem 4. We need to relate solutions of (1.1) to asymptotics of the Stieltjes transform of ρ following Hamburger [8] and Nevanlinna [29].

Proposition 4.13. *Let* $\mathcal{M}^H(\gamma) = \{\rho \mid \rho \text{ obeys } (1.1)\}$*. Let* $G_\rho(z) = \int \frac{d\rho(x)}{x-z}$*. Then for any* N *as* $y \to \infty$*,*

$$y^{N+1}\left[G_\rho(iy) + \sum_{n=0}^{N}(-i)^{n+1}y^{-n-1}\gamma_n\right] \to 0 \tag{4.28}$$

uniformly for ρ *in* $\mathcal{M}^H(\gamma)$*. Conversely, if* G *is a function on* $\mathbb{C}_+$ *with* $\operatorname{Im} G(z) > 0$ *there and so that* (4.28) *holds for each* N*, then* $G(z) = G_\rho(z)$ *for some* ρ *in* $\mathcal{M}^H(\gamma)$*.*

Proof. By the geometric series with remainder, the left side of (4.28) is

$$-(-i)^{N+1}y^{N+1}\int \frac{d\rho(x)}{x-iy}\,\frac{x^{N+1}}{y^{N+1}} \equiv R_N(\rho) \tag{4.29}$$

so, using $|x-iy|^{-1} \le y^{-1}$,

$$|R_N(\rho)| \le y^{-1}\int |x|^{N+1}d\rho(x)\begin{cases} = \gamma_{N+1}y^{-1} & \text{if } N \text{ is odd} \\ \le \frac{1}{2}[\gamma_N + \gamma_{N+2}]y^{-1} & \text{if } N \text{ is even.}\end{cases}$$

This shows that (4.28) holds and the convergence is uniform for $\rho \in \mathcal{M}^H(\gamma)$.

For the converse, first use the Herglotz representative theorem which says that if G maps $\mathbb{C}_+$ to $\mathbb{C}_+$, then for some measure $d\rho$, some $c \ge 0$ and some real d:

$$G(z) = cz + d + \int d\rho(x)\left[\frac{1}{x-z} - \frac{x}{1+x^2}\right], \tag{4.30}$$

where, a priori, ρ only obeys

$$\int \frac{d\rho(x)}{1+x^2} < \infty.$$

By (4.28),

$$y[G(iy)] \to i\gamma_0. \tag{4.31}$$

If (4.30) holds, then $y^{-1}G(iy) \to ic$, so $c = 0$. Since $c = 0$, (4.30) says

$$y \operatorname{Im} G(iy) = \int \frac{y^2}{x^2+y^2}\,d\rho(x),$$

so (4.31) and the monotone convergence theorem implies that $\int d\rho(x) = \gamma_0$. Once this is true, (4.30) implies that as $y \to \infty$,

$$\operatorname{Re} G(iy) \to d - \int d\rho(x)\,\frac{x}{1+x^2} \tag{4.32}$$

so (4.31) implies the right side of (4.32) is zero, and thus (4.30) becomes

$$G(z) = \int \frac{d\rho(x)}{x-z}\,. \tag{4.33}$$

We will now prove inductively that ρ obeys (1.1), that is, $\rho \in \mathcal{M}^H(\gamma)$. Suppose that we know that (1.1) holds for $n = 0, 1, \dots, 2M-2$. (4.28) for $N = 2M$ then implies that

$$\int \frac{(iy)^2 x^{2M-1}}{x - iy}\, d\rho(x) + iy\gamma_{2M-1} \to -\gamma_{2M}.$$

Taking real and imaginary parts, we see that

$$\gamma_{2M-1} = \lim_{y\to\infty} \int \frac{y^2 x^{2M-1}}{x^2+y^2}\, d\rho(x) \tag{4.34}$$

$$\gamma_{2M} = \lim_{y\to\infty} \int \frac{y^2 x^{2M}}{x^2+y^2}\, d\rho(x). \tag{4.35}$$

(4.35) and monotone convergence implies that $\int x^{2M}\, d\rho(x) < \infty$, so that dominated convergence and (4.34), (4.35) imply that (1.1) holds for $n = 0, 1, 2, \dots, 2M$. $\square$

Let $\mathcal{F}$ be the set of analytic maps from $\mathbb{C}_+$ to $\bar{\mathbb{C}}_+ \cup \{\infty\}$. By the open mapping theorem for analytic functions, $\Phi \in \mathcal{F}$ either maps $\mathbb{C}_+$ to $\mathbb{C}_+$ or Φ has a constant value in $\mathbb{R} \cup \{\infty\}$.

Theorem 4.14 (Nevanlinna [29]). *Let γ be a set of indeterminate Hamburger moments. Then there is a one-one correspondence between solutions, ρ, of the moment problem and functions $\Phi \in \mathcal{F}$ given by*

$$G_\rho \equiv \int \frac{d\rho(x)}{x - z} = -\frac{C(z)\Phi(z) + A(z)}{D(z)\Phi(z) + B(z)}\,. \tag{4.36}$$

In particular, if ρ is not a von Neumann solution, $G_\rho(z) \in D(z)^{\mathrm{int}}$ for all $z \in \mathbb{C}_+$.

Remarks. 1. By (4.21), the von Neumann solutions μ_t correspond precisely to the case $\Phi(z) \equiv t \in \mathbb{R} \cup \{\infty\}$.

2. We will call the Herglotz function associated to some $\rho \in \mathcal{M}^H(\gamma)$ the *Nevanlinna function* of ρ and denote it by Φ_ρ. Conversely, given Φ (and γ), we denote by ρ_Φ the associated solution of the moment problem.

3. In Section 6, we will discuss the ρ_Φ's associated to the case where the measure μ in the Herglotz representation (1.19) is a measure with finite support.

Proof. Let $\Phi \in \mathcal{F}$ and let $G(z)$ denote the right side of (4.36). In terms of the map $F(z)$ of (4.27), $G(z) = F(z)(\Phi(z))$, so by Proposition 4.12, $G(z) \in \mathcal{D}(z)$. By the uniformity in Proposition 4.13, the fact that the $\mu_t \in \mathcal{M}^H(\gamma)$ and that $\{G_{\mu_t}(z) \mid t \in \mathbb{R}\cup\{\infty\}\} = \partial\mathcal{D}(z)$, this implies that $G(z)$ obeys (4.28). Thus by Proposition 4.13, $G(z) = G_\rho(z)$ for some $\rho \in \mathcal{M}^H(\gamma)$.

Conversely, let $\rho \in \mathcal{M}^H(\gamma)$ and consider $G_\rho(z)$. By Theorem 4.3, Proposition 4.4 and Proposition 4.12, $\Phi(z) \equiv F(z)^{-1}(G_\rho(z)) \in \bar{\mathbb{C}}_+ \cup \{\infty\}$, and so $\Phi \in \mathcal{F}$. Thus, $G_\rho(z) = F(z)(\Phi(z))$, that is, (4.36) holds.

If ρ is not a von Neumann solution, then $\operatorname{Im}\Phi_\rho(z) > 0$, so $G_\rho(z) = F(z)(\Phi_\rho(z))$ is in the interior of $\mathcal{D}(z)$. $\square$

Proposition 4.15. *Let $\rho \in \mathcal{M}^H(\gamma)$. If ρ is a von Neumann solution, then the polynomials are dense in $L^2(\mathbb{R}, d\rho)$ and for each $z_0 \in \mathbb{C}_+$, there is no other μ in $\mathcal{M}^H(\gamma)$ with $G_\mu(z_0) = G_\rho(z_0)$. If ρ is not a von Neumann solution, then the polynomials are not dense in $L^2(\mathbb{R}, d\rho)$ and for each $z_0 \in \mathbb{C}_+$, there are distinct μ's in $\mathcal{M}^H(\gamma)$ with $G_\mu(z_0) = G_\rho(z_0)$.*

Proof. If ρ is a von Neumann solution, the polynomials are dense by construction and the uniqueness result holds since $G_\mu(z_0) = G_\rho(z_0)$ if and only if $\Phi_\mu(z_0) = \Phi_\rho(z_0)$ and $\Phi_\rho(z_0)$ is then real.

Conversely, suppose ρ is not a von Neumann solution. Then, $G_\rho(z_0) \in D(z)^{\mathrm{int}}$, so by the proof of Theorem 4.3, $(x - z_0)^{-1}$ is not in the L^2 closure of the polynomials. Thus, the polynomials are not dense. If Φ_ρ is not a constant, set $\Psi(z) = -|\Phi_\rho(z_0)|^2 \Phi_\rho(z)^{-1} + 2\mathrm{Re}\,\Phi_\rho(z_0)$. If $\Phi_\rho(z)$ is a constant, q (of necessity with $\mathrm{Im}\, q > 0$), set $\Psi(z) = cz + d$ with $c = \frac{\mathrm{Im}\, q}{\mathrm{Im}\, z_0}$ (> 0) and $d = \mathrm{Re}\, q - c\, \mathrm{Re}\, z_0$. In either case, $\Psi \neq \Phi$, Ψ is Herglotz, and $\Psi(z_0) = \Phi(z_0)$. Thus, if $\mu = \rho_\Psi$, we have $G_\mu(z_0) = F(z_0)(\Psi(z_0)) = F(z_0)(\Phi(z_0)) = G_\rho(z_0)$. $\square$

To complete the proof of Theorem 5, we need the following fact about Herglotz functions:

Theorem 4.16. *Let $\Phi(z)$ be a Herglotz function so*

$$\Phi(z) = cz + d + \int d\mu(x) \left[\frac{1}{x - z} - \frac{x}{1 + x^2} \right]$$

with d real, $c \geq 0$, and either $c > 0$ or $d\mu \neq 0$. Suppose for some x_0, $\Phi(x_0 + i\varepsilon) \to t \in \mathbb{R}$. Then either $|\frac{[\Phi(x_0+i\varepsilon)-t]}{i\varepsilon}| \to \infty$ or else $\int \frac{d\mu(x)}{(x-x_0)^2} < \infty$ and

$$\lim_{\varepsilon \downarrow 0} \frac{\Phi(x_0 + i\varepsilon) - t}{i\varepsilon} = c + \int \frac{d\mu(x)}{(x - x_0)^2}\,. \tag{4.37}$$

Remark. Do not confuse the μ in the Herglotz representation for Φ and the measure ρ of (4.36). In particular, μ is allowed to have finite support even though we are suppposing that ρ does not.

Proof. Note first that

$$\frac{\mathrm{Im}\, \Phi(x_o + i\varepsilon)}{\varepsilon} = c + \int \frac{d\mu(x)}{(x - x_0)^2 + \varepsilon^2}\,. \tag{4.38}$$

On the other hand,

$$\mathrm{Im}\, \frac{\partial \Phi}{\partial z}\, (x_0 + i\varepsilon) = \int \frac{d\mu(x)\, 2\varepsilon(x - x_0)}{[(x - x_0)^2 + \varepsilon^2]^2}\,. \tag{4.39}$$

If $\int \frac{d\mu(x)}{(x-x_0)^2} = \infty$, then (4.38) implies $\mathrm{Im}\, [\frac{\Phi(x_0+i\varepsilon)-t}{\varepsilon}] \to \infty$, so if the limit is finite, then $\int \frac{d\mu(x)}{(x-x_0)^2} < \infty$. (4.39) and the dominated convergence theorem implies that $\mathrm{Im}\, \frac{\partial\Phi}{\partial z}(x_0 + i\varepsilon) \to 0$ so that $\frac{[\mathrm{Re}\, \Phi(x_0+i\varepsilon)-t]}{i\varepsilon} = \frac{1}{\varepsilon} \int_0^\varepsilon \mathrm{Im}\, \frac{\partial\Phi}{\partial z}(x_0 + iy)\, dy \to 0$. This and (4.38) implies (4.37). $\square$

Theorem 4.17 (end of Theorem 5). *Let γ be an indeterminate moment problem. Let $\rho \in \mathcal{M}^H(\gamma)$ correspond to a Φ which is not a constant in $\mathbb{R} \cup \{\infty\}$ (so that ρ is not a von Neumann solution). Suppose $\alpha \equiv \rho(\{x_0\}) > 0$ for some point $x_0 \in \mathbb{R}$. Then there is a von Neumann solution μ_t so that $\mu_t(\{x_0\}) > \alpha$.*

Proof. We will suppose that $D(x_0) \neq 0$. If $D(x_0) = 0$, then $B(x_0) \neq 0$ and we can use

$$-\frac{C(z)\Phi(z) + A(z)}{D(z)\Phi(z) + B(z)} = -\frac{A(z)(-\Phi(z))^{-1} - C(z)}{B(z)(-\Phi(z))^{-1} - D(z)}$$

and $-\Phi(z)^{-1}$ in place of $\Phi(z)$ to give an identical argument. Define $t = -\frac{B(x_0)}{D(x_0)} \in \mathbb{R}$. Since $AD - BC = 1$,

$$C(x_0)t + A(x_0) = \frac{1}{D(x_0)} \tag{4.40}$$

is non-zero and has the same sign as D.

$$(-i\varepsilon)G_\rho(x_0 + i\varepsilon) = (i\varepsilon)\left[\frac{C(x_0 + i\varepsilon)\Phi(x_0 + i\varepsilon) + A(x_0 + i\varepsilon)}{D(x_0 + i\varepsilon)\Phi(x_0 + i\varepsilon) + B(x_0 + i\varepsilon)}\right] \to \alpha.$$

This is only possible if $G_\rho(x_0 + i\varepsilon) \to \infty$, which requires that $\Phi(x_0 + i\varepsilon) \to t$. Then

$$C(x_0 + i\varepsilon)\Phi(x_0 + i\varepsilon) + A(x_0 + i\varepsilon) \to C(x_0)t + A(x_0)$$

while

$$\frac{D(x_0 + i\varepsilon)\Phi(x_0 + i\varepsilon) + B(x_0 + i\varepsilon)}{i\varepsilon} \to D'(x_0)t + B'(x_0) + D(x_0)\lim_{\varepsilon \downarrow 0} \frac{\Phi(x_0 + i\varepsilon) - t}{i\varepsilon}.$$

Thus using (4.40),

$$\alpha = \frac{1}{D(x_0)^2 \lim_{\varepsilon \downarrow 0} \frac{\Phi(x_0 + i\varepsilon) - t}{i\varepsilon} + D(x_0)[D'(x_0)t + B'(x)]}.$$

On the other hand, taking $\Phi(x) \equiv t$ to describe μ_t,

$$\mu_t(\{x_0\}) = \frac{1}{D(x_0)[D'(x_0)t + B'(x_0)]}$$

must be positive. It follows from Lemma 4.16 that $\int \frac{d\mu(x)}{(x - x_0)^2} < \infty$ and that

$$\alpha^{-1} > \mu_t(\{x_0\})^{-1}. \quad \square$$

Finally, we turn to the Nevanlinna parametrization in the indeterminate Stieltjes case. As we have seen, among the B_t there are two distingtuished ones, B_F and B_K. The Krein extension has $\ker(A^*) \subset D(B_K)$ so $\pi(0) \in D(B_K)$, which means $t = \infty$ in the notation of (4.20). The Friedrichs extension is $B_F = B_{t_0}$ where $t_0 = (\delta_0, A_F^{-1}\delta_0)$.

Theorem 4.18 (Stieltjes case of Theorem 4). *If the Stieltjes problem for γ is indeterminate, its solutions obey* (4.36) *for precisely those Φ that either are a constant in $[t_0,\infty)\cup\{\infty\}$ or that obey $\Phi(z)$ is analytic in $\mathbb{C}\backslash[0,\infty)$ with $\Phi(x)\in[t_0,\infty)$ if $x\in(-\infty,0)$. Here $t_0=(\delta_0,A_F^{-1}\delta_0)$.*

Remark. Such Φ's are precisely those of the form

$$\Phi(z)=d+\int_0^\infty \frac{d\mu(x)}{x-z}\,, \tag{4.41}$$

where $d\geq t_0$ and $\int_0^\infty \frac{d\mu(x)}{x+1}<\infty$.

Proof. Clearly, the solutions of the Stieltjes problem are precisely the solutions ρ of the Hamburger problem with $\lim_{\varepsilon\downarrow 0} G_\rho(-y+i\varepsilon)$ real for each $y\in(0,\infty)$. Since the B_t's obey $t=(\delta_0,B_t^{-1}\delta_0)$ and $B_K<B_t<B_F$ means $t_0<(\delta_0,B_t^{-1}\delta_0)<\infty$, we know that for $y\in(-\infty,0)$, $F(y)$ maps $[t_0,\infty)$ into $(0,\infty)$ ($F(\,\cdot\,)$ is given by (4.27)). It follows that if Φ obeys $\Phi(x)\in[t_0,\infty)$ for $x\in(-\infty,0)$, then $G_\rho(y+i\varepsilon)$ has a limit in $(0,\infty)$ on $(-\infty,0)$, that is, Φ defines a solution of the Stieltjes moment problem. The converse follows from this argument and the next theorem. □

Theorem 4.19. *Let $d\mu_F$ and $d\mu_K$ be the Friedrichs and Krein solutions of an indeterminate Stieltjes moment problem and let $d\rho$ be another solution. Then for all $y\in(0,\infty)$,*

$$\int_0^\infty \frac{d\mu_F(x)}{x+y}\leq\int_0^\infty \frac{d\rho(x)}{x+y}\leq\int_0^\infty \frac{d\mu_K(x)}{x+y}\,. \tag{4.42}$$

This will be proven below as part of Theorem 5.2.

Corollary 4.20. *If $\rho\in\mathcal{M}^S(\gamma)$ and $d\rho\neq d\mu_F$, then for $y\in[0,\infty)$,*

$$\int_0^\infty \frac{d\mu_F(x)}{x+y}<\int_0^\infty \frac{d\rho(x)}{x+y}\,. \tag{4.43}$$

(*Note that the inequality is strict.*)

Proof. For each $y\in(0,\infty)$, $F(-y)(\,\cdot\,)$ is a strictly monotone map of $[t_0,\infty)$ to $[G_{\mu_F}(-y),$ $G_{\mu_K}(-y))$ by the proof of Theorem 4.18 and the fact that any fractional linear map of $\mathbb{R}$ to $\mathbb{R}$ is monotone in any region where it is finite. By a limiting argument, the same is true for $y=0$. Thus, (4.43) follows from the relation of Nevanlinna functions $\Phi_\rho(y)>\Phi_{\mu_F}(y)\equiv t_0$. This is immediate from (4.41). □

As a corollary of this, we see

Corollary 4.21. *Let γ be a set of indeterminate Stieltjes moments and let $d\mu_F$ be its Friedrichs solution. Let $r=\int x^{-1}d\mu_F(x)$ and let*

$$\tilde\gamma_0=1;\qquad \tilde\gamma_n=r^{-1}\gamma_{n-1},\qquad n=1,2,\ldots.$$

Then $\{\tilde{\gamma}_j\}_{j=0}^{\infty}$ *is a determinate Hamburger moment problem.*

Remark. This lets us produce Stieltjes determinate moment problems with essentially arbitrary rates of growth for γ_n. By using Theorem 2.13, we obtain determinate Hamburger problems with arbitrary fast growth also.

Proof. $r^{-1}x^{-1}d\mu_F \equiv d\lambda_0(x)$ is a Stieltjes measure whose moments are $\tilde{\gamma}$. Let $d\lambda(x)$ be another such Stieltjes measure and let $d\rho(x) = rx\, d\lambda(x)$. Then the moments of $d\rho$ are γ and $\int x^{-1}d\rho(x) = r$. So, by Corollary 4.20, $\rho = \mu_F$. Thus, $\lambda = \lambda_0$. Thus, λ_0 is the unique solution of the Stieltjes problem. But $0 \notin \operatorname{supp}(d\lambda_0)$. Thus by Proposition 3.1, the Hamburger problem is also determinate. $\square$

§5. Padé Approximants, Continued Fractions, and Finite Matrix Approximations

In this section, we will primarily consider aspects of the Stieltjes moment problem. We will discuss finite matrix approximations which converge to the Friedrichs and Krein extensions of A and, as a bonus, obtain Theorem 4.19 and Theorems 5, 6, 7, and 8. We will see that the convergence of the Padé approximants (equivalently, continued fractions of Stieltjes) can be reinterpreted as strong resolvent convergence of certain finite matrix approximations to A_F and A_K.

Before we start, we note that our continued fraction expressions are related to but distinct from those of Stieltjes. Our basic object (the approximations to A_F) are of the form:

$$\cfrac{1}{-z+b_0-\cfrac{a_0^2}{-z+b_1-\cfrac{a_1^2}{-z+b_2+\cdots}}} \tag{5.1a}$$

with two terms (an affine polynomial) at each stage while Stieltjes' are of the form

$$\cfrac{1}{c_1w+\cfrac{1}{c_2+\cfrac{1}{c_3w+\cdots}}} \tag{5.1b}$$

with a single term in each step and alternate constant and linear terms. This gives him twice as many continued fractions, so his alternate between the two sets of rational approximations we get. We will say more about this later.

Until Theorem 5.29 below, we will suppose $\{\gamma_n\}_{n=0}^{\infty}$ is a set of Stieltjes moments.

Given the Jacobi matrix (1.16), we will consider two $N \times N$ approximations. The first

is obvious:

$$A_F^{[N]} = \begin{pmatrix} b_0 & a_0 & & & \\ a_0 & b_1 & & & \\ & & \ddots & & \\ & & & b_{N-2} & a_{N-2} \\ & & & a_{N-2} & b_{N-1} \end{pmatrix}. \tag{5.2a}$$

The second differs by the value of the NN coefficient:

$$A_K^{[N]} = \begin{pmatrix} b_0 & a_0 & & & \\ a_0 & b_1 & & & \\ & & \ddots & & \\ & & & b_{N-2} & a_{N-2} \\ & & & a_{N-2} & b_{N-1} - \alpha_{N-1} \end{pmatrix}, \tag{5.2b}$$

where α_{N-1} is chosen so that $A_K^{[N]}$ has a zero eigenvalue. That such an α_{N-1} exists is the content of

Lemma 5.1. *There is a unique* $\alpha_{N-1} > 0$ *so that* (5.2b) *has a zero eigenvalue.* $A_K^{[N]} \geq 0$ *and* α_{N-1} *obeys*

$$(b_{N-1} - \alpha_{N-1})P_{N-1}(0) + a_{N-2}P_{N-2}(0) = 0 \tag{5.3}$$

and

$$\alpha_{N-1} = -a_{N-1}\,\frac{P_N(0)}{P_{N-1}(0)}\,. \tag{5.4}$$

Moreover,

$$(b_N - \alpha_N)(\alpha_{N-1}) - a_{N-1}^2 = 0. \tag{5.5}$$

Proof. Any solution of $A_K^{[N]}u = 0$ must obey the eigenfunction equation (4.1) and so be a multiple of $P_j(0)$, that is,

$$u_j = P_j(0), \qquad j = 0, 1, \dots, N-1.$$

This obeys the condition at the lower right of the matrix if and only if (5.3) holds.

If $P_{N-1}(0)$ were 0, then $A_F^{[N-1]}$ would have a zero eigenvalue, which is impossible since $A_F^{[N-1]}$ is strictly positive definite (since the form S_{N-1} is strictly positive definite). Thus, $P_{N-1}(0) \neq 0$ and so (5.3) has a unique solution. Since $A_F^{[N]}$ is positive definite, this solution must have $\alpha_{N-1} > 0$.

The eigenfunction equation for $P_N(0)$ then yields (5.4). (5.3) for $N \to N+1$ and (5.4) yield two formulas for $\frac{P_N(0)}{P_{N-1}(0)}$. Setting these to each other yields (5.5). $\square$

The first main result of this section, towards which we are heading, is

Theorem 5.2 (includes Theorem 4.19). *Let*

$$f_N^+(z) \equiv (\delta_0, (A_K^{[N]} - z)^{-1}\delta_0) \tag{5.6}$$

and

$$f_N^-(z) \equiv (\delta_0, (A_F^{[N]} - z)^{-1}\delta_0). \tag{5.7}$$

Then for $x \in (0, \infty)$,

$$f_N^+(-x) \geq f_{N+1}^+(-x) \text{ converges to } (\delta_0, (A_K + x)^{-1}\delta_0) \equiv f^+(-x)$$

while

$$f_N^-(-x) \leq f_{N+1}^-(-x) \text{ converges to } (\delta_0, (A_F + x)^{-1}\delta_0) \equiv f^-(-x).$$

The convergence holds for any $z \in \mathbb{C}\backslash[0, \infty)$ and is uniform on compacts. Moreover, for any solution ρ of the moment problem and $x > 0$,

$$f^-(-x) \leq \int \frac{d\rho(y)}{x + y} \leq f^+(-x). \tag{5.8}$$

Remarks. 1. Notice that (5.8) is (4.42).

2. Let $A^{[N]}(\beta)$ be (5.2b) with α_{N-1} replaced by $-\beta$. Then $A_K^{[N]}$ is quite a natural approximation: It is that $A^{[N]}(\beta)$ which is minimal among the non-negative matrices — reasonable to capture A_K, the minimal non-negative self-adjoint extension. From this point of view, $A_F^{[N]}$ seems less natural. One would instead want to consider $\lim_{\beta\to\infty} A^{[N]}(\beta)$. In fact, one can show this limit is "essentially" $A_F^{[N-1]}$ in the sense that

$$\lim_{\beta\to\infty} (\delta_0, (A^{[N]}(\beta) - z)^{-1}\delta_0) = (\delta_0, (A_F^{[N-1]} - z)^{-1}\delta_0).$$

Thus, the $A^{[N]}(\beta)$ interpolate between $A_K^{[N]}$ and $A_F^{[N-1]}$.

Proposition 5.3. *Let $\tilde{A}_K^{[N]}$ be the operator on ℓ^2 which is $A_K^{[N]} \oplus 0$. Then $\tilde{A}_K^{[N]}$ converges to A_K in strong resolvent sense.*

Remark. For self-adjoint operators $\{A_n\}_{n=1}^\infty$ and A_∞, we say A_n converges to A_∞ in strong resolvent sense if and only if for all $z \in \mathbb{C}\backslash\mathbb{R}$, $(A_n - z)^{-1}\varphi \to (A_\infty - z)^{-1}\varphi$ for all vectors φ. It is a basic theorem (see Reed-Simon [33]) that it suffices to prove this for a single $z \in \mathbb{C}\backslash\mathbb{R}$. The same proof shows that if all A_n and A_∞ are non-negative, one then also has convergence for $z \in (-\infty, 0)$. Moreover, one has convergence uniformly for z in compact subsets of $\mathbb{C}\backslash[0, \infty)$.

Proof. Suppose first that the Hamburger problem is indeterminate. Thus, $\pi(0) = (P_0(0), \dots) \in \ell_2$. Let $P^{[n]}(0)$ be the vector $(P_0(0), \dots, P_{n-1}(0), 0, 0, \dots)$. Then $A_K^{[n]} P^{[n]}$

$= 0$ so $(A_K^{[n]} - z)^{-1} P^{[n]} = -z^{-1} P^{[n]}$ for any $z \in \mathbb{C} \backslash \mathbb{R}$. Since $\|(A_K^{[n]} - z)^{-1}\| \le |\mathrm{Im}\, z|^{-1}$ for any such z, and $\|P^{[n]} - \pi(0)\| \to 0$, we conclude that

$$(A_K^{[n]} - z)^{-1}\pi(0) \to -z^{-1}\pi(0) = (A_K - z)^{-1}\pi(0) \tag{5.9}$$

since $A_K\pi(0) = 0$.

Suppose $\varphi = (A - z)\eta$ for $\eta \in D(A)$, that is, a finite sequence. Then $(A_K - z)\eta = \varphi = (A_K^{[n]} - z)\eta$ for n large, and thus $\lim_{n\to\infty}(A_K^{[n]} - z)^{-1}\varphi = \eta = (A_K - z)^{-1}\varphi$. Thus, $(A_K^{[n]} - z)^{-1}\varphi \to (A - z)^{-1}\varphi$ for $\varphi \in \overline{\mathrm{Ran}(A - z)}$. In the determinate case, that is all φ's; while in the indeterminate case, we claim that $\overline{\mathrm{Ran}(A - z)} + [\pi(0)]$ is all of ℓ^2 so (5.9) completes the proof.

That leaves the proof of our claim that $\overline{\mathrm{Ran}(A - z)} + [\pi(0)]$ is ℓ^2. We first note that $\pi(0) \notin D(\bar{A})$ by Proposition 4.4. $(A_K - z)^{-1}(\overline{\mathrm{Ran}(A - z)} + [\pi(0)]) = D(\bar{A}) + [\pi(0)]$ since $(A_K - z)^{-1})\pi(0) = -z^{-1}\pi(0)$. But $D(A_K)/D(\bar{A})$ has dim 1 and $\pi(0) \notin D(\bar{A})$ so $(A_K - z)^{-1}(\overline{\mathrm{Ran}(A - z)} + [\pi(0)]) = D(A_K)$ and thus, since $\mathrm{Im}\, z \neq 0$, $\overline{\mathrm{Ran}(A - z)} + [\pi(0)] = \ell_2$, as claimed. $\square$

Proposition 5.4. *Let $\tilde{\tilde{A}}_K^{[N]}$ be the $(N+1) \times (N+1)$ matrix which is $A_K^{[N]} \oplus 0$, that is, it has zeros in its last row and column. Then*

$$\tilde{\tilde{A}}_K^{[N]} \le A_K^{[N+1]}. \tag{5.10}$$

In particular, for $x > 0$,

$$(\delta_0, (A_K^{[N+1]} + x)^{-1}\delta_0) \le (\delta_0, (\tilde{\tilde{A}}_K^{[N]} + x)^{-1}\delta_0) = (\delta_0, (A_K^{[N]} + x)^{-1}\delta_0).$$

Remark. Propositions 5.3 and 5.4 prove the part of Theorem 5.2 involving monotonicity of f_N^+ and its convergence.

Proof. $B \equiv A_K^{[N+1]} - \tilde{\tilde{A}}_K^{[N]}$ is an $(N+1) \times (N+1)$ matrix which has all zeros except for a 2×2 block in its lower right corner. This block is

$$\begin{pmatrix} \alpha_{N-1} & a_{N-1} \\ a_{N-1} & b_N - \alpha_N \end{pmatrix},$$

which is symmetric with a positive trace and determinant zero (by (5.5)). Thus, the block is a positive rank one operator so B is positive, proving (5.10). $\square$

The monotonicity of the $A_F^{[N]}$'s and their convergence is a special case of monotone convergence theorems for forms. Consider non-negative closed quadratic forms whose domain may not be dense. Each such form q_B with $D(q_B)$ is associated to a non-negative self-adjoint operator B on $\overline{D(q_B)}$. We define $(B - x)^{-1}$ to be 0 on $D(q_B)^\perp$. This essentially sets $B = \infty$ on $D(q_B)^\perp$ consistent with the intention that $D(q_B)$ is the set of φ for which $q_B(\varphi) < \infty$.

Given two forms q_B and q_C, we say $q_B \leq q_C$ if and only if $D(q_B) \supseteq D(q_C)$ (intuitively $q_C(\varphi) < \infty$ implies $q_B(\varphi) < \infty$) and for all $\varphi \in q_C$, $q_C(\varphi) \geq q_B(\varphi)$. It is a fundamental result [12, 37] that if $q_B \leq q_C$, then for all $x \geq 0$ and all φ,

$$(\varphi, (C+x)^{-1}\varphi) \leq (\varphi, (B+x)^{-1}\varphi). \tag{5.11}$$

One monotone convergence theorem for forms [12, 37] says the following: Let $\{q_{A_n}\}_{n=1}^{\infty}$ be a sequence of quadratic forms with $q_{A_n} \geq q_{A_{n+1}}$. Then $(A_n + x)^{-1}$ converges to the resolvent, $(A_\infty + x)^{-1}$, of an operator A_∞. It is the operator associated to the form q_{A_∞} defined to be the closure of $\tilde{q}_{A_\infty}$ where $D(\tilde{q}_{A_\infty}) = \cup D(q_{A_n})$ with $\tilde{q}_{A_\infty}(\varphi) = \lim_{n\to\infty} q_{A_n}(\varphi)$ provided that the form $\tilde{q}_{A_\infty}$ is closable.

We can apply this to the $A_F^{[N]}$. Let $q_F^{[N]}$ be defined to be the form with $D(q_F^{[N]}) = \{(\varphi_0, \dots, \varphi_{N-1}, 0, \dots, 0, \dots)\}$ and $q_F^{[N]}(\varphi) = (\varphi, A\varphi)$. Then $D(q_F^{[N]}) \subset D(q_F^{[N+1]})$ and $q_F^{[N]}(\varphi) = q_F^{[N+1]}(\varphi)$ if $\varphi \in D(q_F^{[N]})$. Thus, $q_F^{[N]} \geq q_F^{[N+1]}$ (in essence, $\tilde{A}_F^{[N]} = A_F^{[N]} \oplus \infty$ on $\mathbb{C}^{N+1}$). The monotone convergence theorem applies. A_∞ is just the closure of $\varphi \mapsto (\varphi, A\varphi)$ on finite sequences, that is, the Friedrichs extension A_F, so we have the convergence and monotonicity part of Theorem 5.2 for f_N^- (using (5.11)):

Proposition 5.5. *Let $x > 0$. Then $(\delta_0, (A_F^{[N+1]} + x)^{-1}\delta_0) \geq (\delta_0, (A_F^{[N]} + x)^{-1}\delta_0)$ and this converges to $(\delta_0, (A_F + x)^{-1}\delta_0)$ as $N \to \infty$.*

To head towards the remaining part of Theorem 5.2, viz. (5.8), we need expressions for $(\varphi, (A_F^{[N]} - z)^{-1}\varphi)$ and $(\varphi, (A_K^{[N]} - z)^{-1}\varphi)$, which are of independent interest.

Proposition 5.6.

$$(\delta_0, (A_F^{[N]} - z)^{-1}\delta_0) = -\frac{Q_N(z)}{P_N(z)} \tag{5.12}$$

Proof. The only possible eigenfunctions of $A_F^{[N]}$ are the vectors $\pi^{[N]}(z) \equiv (P_0(z), \dots, P_{N-1}(z))$. By the eigenfunction equation (4.1), this is an eigenfunction of $A_F^{(N)}$ if and only if $P_N(z) = 0$. Thus, the N poles of $(\delta_0, (A_F^{[N]} - z)^{-1}\delta_0)$ are precisely the N-zeros of $P_N(z)$. The zeros are distinct because the eigenvalues are simple (since $\pi^{[N]}(z)$ is the only potential eigenfunction, since eigenfunctions must have $u_0 \neq 0$).

Now let the $B_F^{[N]}$ be the $(N-1) \times (N-1)$ matrix obtained by removing the top row and left column of $A_F^{[N]}$. By Cramer's rule, $(\delta_0, (A_F^{[N]} - z)^{-1}\delta_0) = \frac{\det(B_F^{[N]} - z)}{\det(A_F^{[N]} - z)}$, so the $N-1$ zeros of $(\delta_0, (A_F^{[N]} - z)^{-1}\delta_0)$ are precisely the $N-1$ eigenvalues of $B_F^{[N]}$. The only possible eigenfunctions of $B_F^{[N]}$ are $\xi(z)^{[N-1]} = (Q_1(z), \dots, Q_{N-1}(z))$ (since $Q_0(z) = 0$, $Q_1(z) = \frac{1}{a_0}$). Thus, the eigenvalues of $B_F^{[N]}$ are precisely z's with $Q_N(z) = 0$. It follows that

$$(\delta_0, (A_F^{[N]} - z)^{-1}\delta_0) = \frac{d_N Q_N(z)}{P_N(z)}\,,$$

and we need only show that $d_N \equiv -1$.

Since $(\delta_0, (A_F^{[N=1]} - z)^{-1}\delta_0) = (b_0 - z)^{-1}$ and $Q_1(z) = \frac{1}{a_0}$, $P_1(z) = \frac{(z-b_0)}{a_0}$, we see that $d_1 = -1$. On the other hand, Proposition 4.1 implies that

$$\frac{Q_k(z)}{P_k(z)} - \frac{Q_{k-1}(z)}{P_{k-1}(z)} = \frac{1}{a_{k-1}P_k(z)P_{k-1}(z)} = o\left(\frac{1}{z}\right).$$

Moreover, $(\delta_0, (A - z)^{-1})\delta_0) = -z^{-1} + O(z^{-2})$, so $d_k = d_{k-1}$, that is, $d_N = -1$ for all N. $\square$

Remarks. 1. The proof shows that for suitable c_N (indeed, an induction shows that $c_N = (-1)^N(a_0 \dots a_{N-1})^{-1}$), we have

$$P_N(z) = c_N \det(A_F^{[N]} - z) \tag{5.13}$$

and

$$Q_N(z) = -c_N \det(B_F^{[N]} - z). \tag{5.14}$$

2. Since $A_F^{[N]}$ is strictly positive definite, (5.13) shows once more that $P_N(0) \neq 0$ in the Stieltjes case. Since $B_F^{[N]}$ is also strictly positive definite (as a submatrix of $A_F^{[N]}$), (5.14) shows that $Q_N(0) \neq 0$ also in the Stieltjes case.

(5.13)–(5.14) imply some facts about the zeros of P_N and Q_N:

Proposition 5.7. *All the zeros of each $P_N(z)$ and each $Q_N(z)$ are real. Moreover, there is exactly one zero of $Q_N(z)$ and one zero of $P_{N-1}(z)$ between any pair of successive zeros of $P_N(z)$.*

Proof. The first assertion follows from the fact that the eigenvalues of a real-symmetric matrix are all real. The second assertion follows from the fact that if X is an $N \times N$ real-symmetric matrix and Y is an $N - 1 \times N - 1$ submatrix, then by the min-max principle, there is exactly one eigenvalue of Y between any pair of eigenvalues of X. $\square$

Remark. Since the Q_N's are orthogonal polynomials for another moment problem (see Proposition 5.16), between any two successive zeros of $Q_N(z)$, there is a single zero of $Q_{N-1}(z)$.

Now define

$$M_N(z) = P_N(z) - P_N(0)\,\frac{P_{N-1}(z)}{P_{N-1}(0)} \tag{5.15}$$

$$N_N(z) = Q_N(z) - P_N(0)\,\frac{Q_{N-1}(z)}{P_{N-1}(0)} \tag{5.16}$$

since $A_F^{[j]}$ is strictly positive, 0 is never an eigenvalue and $P_j(0) \neq 0$ for all j, so M is well-defined. Notice $M_N(0) = 0$.

Proposition 5.8.

$$(\delta_0, (A_K^{[N]} - z)^{-1}\delta_0) = -\frac{N_N(z)}{M_N(z)} \tag{5.17}$$

Proof. Let c_N be the constant in (5.13) and let $B_K^{[N]}$ be $A_K^{[N]}$ with the top row and left-most column removed. We will prove that

$$M_N(z) = c_N \det(A_K^{[N]} - z); \qquad N_N(z) = -c_N \det(B_K^{[N]} - z), \tag{5.18}$$

from which (5.17) holds by Cramer's rule.

Clearly,

$$\det(A_K^{[N]} - z) = \det(A_F^{[N]} - z) - \alpha_{N-1} \det(A_F^{[N-1]} - z)$$

so

$$c_N \det(A_K^{[N]} - z) = P_N(z) - \beta_N P_{N-1}(z),$$

where

$$\beta_N = \alpha_{N-1} \, \frac{c_N}{c_{N-1}} \, .$$

But $\det(A_K^{[N]}) = 0$ by construction. So $P_N(0) - \beta_N P_{N-1}(0) = 0$ and thus, $c_N \det(A_K^{[N]} - z) = M_N(z)$.

In the same way,

$$c_N \det(B_K^{[N]} - z) = -Q_N(z) + \beta_N Q_{N-1}(z) = -N_N(z). \quad \square$$

Because of our convergence theorem, we have

Corollary 5.9. *Let* $\{\lambda_i^{[N]}\}_{i=1}^N$ *be the zeros of* $P_N(z)$ *and let* $\nu_i^{[N]} = -\frac{Q_N(\lambda_i^{[N]})}{P_N'(\lambda_i^{[N]})}$. *Then* $\sum_{i=1}^N \nu_i^{[N]} \delta(\lambda - \lambda_i^{[N]})$ *converges to* $d\mu_F(\lambda)$*, the Friedrichs solution of the moment problem. A similar formula holds for the Krein solution,* $d\mu_K(\lambda)$*, with* P, Q *replaced by* M, N*.*

The following concludes the proof of Theorem 5.2. It extends the calculation behind (4.4):

Theorem 5.10. *Let* $d\rho$ *solve the Stieltjes moment problem. Then for* $x > 0$ *and* $N \geq 1$*,*

$$-\frac{Q_N(-x)}{P_N(-x)} \leq \int \frac{d\rho(y)}{x+y} \leq -\frac{N_N(-x)}{M_N(-x)} \, . \tag{5.19}$$

Proof. $\frac{P_N(y) - P_N(z)}{y-z}$ is a polynomial in y of degree $N-1$ so

$$\int d\rho(y) P_N(y) \left[\frac{P_N(y) - P_N(z)}{y - z} \right] = 0. \tag{5.20}$$

On the other hand, (4.4) says that

$$\int d\rho(y)\,\frac{P_N(y)}{y-z} = P_N(z)\int\frac{d\rho(y)}{y-z} + Q_N(z). \tag{5.21}$$

Thus for $z=-x$ with $x>0$,

$$0 \le \int \frac{d\rho(y)P_N^2(y)}{y+x} = P_N(-x)\int\frac{d\rho(y)P_N(y)}{y+x} = P_N(-x)^2\int\frac{d\rho(y)}{x+y} + Q_N(-x)P_N(-x).$$

Dividing by $P_N(-x)^2$, we obtain the left-most inequality in (5.19).

Similarly, since $M_N(0)=0$, $\frac{M_N(z)}{z}$ is a polynomial of degree $N-1$ and so $[y^{-1}M_N(y)-z^{-1}M_N(z)]/y-z$ is a polynomial of degree $N-2$ in y, which is orthogonal to $P_N(y)$ and $P_{N-1}(y)$ and so to $M_N(y)$. Thus

$$\int d\rho(y)\,\frac{M_N(y)}{y-z}\left[\frac{M_N(y)}{y} - \frac{M_N(z)}{z}\right] = 0. \tag{5.22}$$

Since for $N\ge 0$,

$$Q_N(z) = \int d\rho(y)\,\frac{P_N(y)-P_N(z)}{y-z} \tag{5.23}$$

for each z, we see that for $N\ge 1$,

$$N_N(z) = \int d\rho(y)\,\frac{M_N(y)-M_N(z)}{y-z}\,. \tag{5.24}$$

Therefore, for $x>0$,

$$\begin{aligned}0 \le \int \frac{d\rho(y)}{y+x}\;\frac{M_N(y)^2}{y} &= \frac{M_N(-x)}{(-x)}\int d\rho(y)\,\frac{M_N(y)}{y+x} \qquad \text{by (5.22))}\\ &= \frac{M_N(-x)^2}{(-x)}\int\frac{d\rho(y)}{x+y} + \frac{M_N(-x)N_N(-x)}{(-x)}\,.\end{aligned}$$

Dividing by $\frac{M_N(-x)^2}{x}$, we obtain the second half of (5.19). $\square$

Next, we turn to Theorem 6 and the connection of Padé approximants to these finite matrix approximations. Given a formal power series $\sum_{n=0}^\infty \kappa_n z^n$, we define the Padé approximants $f^{[N,M]}(z)$ as follows (see Baker and Graves-Morris [4] for background on Padé approximants): We seek a function $f^{[N,M]}(z)$ so that

$$f^{[N,M]}(z) = \frac{A^{[N,M]}(z)}{B^{[N,M]}(z)}\,, \tag{5.25}$$

where $A^{[N,M]}(z)$ is a polynomial of degree at most N, $B^{[N,M]}(z)$ is a polynomial of degree at most M, as $z \to 0$,

$$f^{[N,M]}(z) - \sum_{j=0}^{N+M} \kappa_j z^j = O(z^{N+M+1}) \tag{5.26}$$

and

$$B^{[N,M]}(0) = 1. \tag{5.27}$$

There is at most one solution, f, for these equations since if $\tilde{A}, \tilde{B}$ are another pair of such polynomials, by (5.26), $\tilde{A}B - A\tilde{B} = O(z^{N+M+1})$ must be zero since $\tilde{A}B - A\tilde{B}$ is a polynomial of degree $N+M$. Thus,

$$A^{[N,M]}(z)\tilde{B}^{[N,M]}(z) - \tilde{A}^{[N,M]}(z)B^{[N,M]}(z) = 0. \tag{5.28}$$

This implies $A/B = \tilde{A}/\tilde{B}$, showing f is uniquely determined as an analytic function. If

$$\deg A = N, \qquad \deg B = M, \qquad A, B \text{ relatively prime,} \tag{5.29}$$

then (5.28) shows $\tilde{A} = A$ and $\tilde{B} = B$, so A and B are uniquely determined. It can be shown ([4]) that if

$$\det((\kappa_{N-M+i+j-1})_{1 \le i,j \le M}) \neq 0 \tag{5.30}$$

then A, B exist and obey (5.29).

There are degenerate cases where a Padé approximant exists, but A, B are not unique (e.g., for $\sum_{n=0}^{\infty} \kappa_n z^n = 1 + z$, $f^{[2,1]}(z) = 1 + z$ can be written as $A(z) = (1+z)(1+\alpha z)$, $B(z) = (1 + \alpha z)$ for any α). In any event, if a solution of (5.25)–(5.27) exists, we say the $[N, M]$ Padé approximant exists and denote it by $f^{[N,M]}(z)$.

In the context of Theorem 6, we are interested in the Padé approximants for the Taylor series of

$$f(z) = \int_0^\infty \frac{d\rho(x)}{1 + zx}\,, \tag{5.31}$$

where ρ is a measure with finite moments. Without loss, normalize ρ so $\int d\rho = 1$. Recall the context of Theorem 6. We have

$$\kappa_n = (-1)^n \int_0^\infty x^n \, d\rho(x)$$

and want to formally sum near $z = 0$:

$$f(z) \sim \sum_{n=0}^{\infty} \kappa_n z^n.$$

If we define
$$\gamma_n = \int_0^\infty x^n \, d\rho(x),$$
then near $w = \infty$,
$$G_\rho(w) \equiv \int_0^\infty \frac{d\rho(x)}{x-w} \sim -\sum_{n=0}^\infty \gamma_n w^{-n-1}. \tag{5.32}$$

Thus formally,
$$f(z) = \frac{1}{z}\, G_\rho\biggl(-\frac{1}{z}\biggr). \tag{5.33}$$

We begin by noting:

Proposition 5.11. *As* $|w| \to \infty$,

$$-\frac{Q_N(w)}{P_N(w)} = -\sum_{j=0}^{2N-1} \gamma_j w^{-j-1} + O(w^{-2N-1}) \tag{5.34}$$
$$-\frac{N_N(w)}{M_N(w)} = -\sum_{j=0}^{2N-2} \gamma_j w^{-j-1} + O(w^{-2N}) \tag{5.35}$$

Proof. Let A be the Jacobi matrix for the moment problem $\{\gamma_n\}_{n=0}^\infty$. Then
$$\gamma_n = \langle \delta_0, A^n \delta_0 \rangle. \tag{5.36}$$

On the other hand, we have an expansion converging near infinity for
$$\langle \delta_0, (A_F^{[N]} - w)^{-1} \delta_0 \rangle = -\sum_{j=0}^\infty (\delta_0, (A_F^{[N]})^j \delta_0) w^{-j-1},$$
so (5.34) follows from
$$\langle \delta_0, (A_F^{[N]})^j \delta_0 \rangle = \langle \delta_0, A^j \delta_0 \rangle, \qquad j = 0, 1, \dots, 2N-1. \tag{5.37}$$

To prove (5.37), note that
$$(A_F^{[N]})^j \delta_0 = A_F^j \delta_0 \tag{5.38}$$
if $j = 0, \dots, N-1$ and for B symmetric,
$$\langle \delta_0, B^{2j} \delta_0 \rangle = \|B^j \delta_0\|$$
and that
$$\langle \delta_0, B^{2j+1} \delta_0 \rangle = \langle B^j \delta_0, B(B^j \delta_0) \rangle. \tag{5.39}$$

To obtain (5.35), note that if $A_F^{[N]}$ is replaced by $A_K^{[N]}$, (5.38) still holds for $j = 0, \dots, N-1$, but (5.39) fails for $j = N-1$ and so the analog of (5.37) only holds for $j = 0, \dots, 2N-2$. $\square$

Remark. While (5.37) holds for $j = 0, 1, 2, \dots, 2N-1$, it never holds for $j = 2N$. For if it did, we would have for any polynomial, R, of degree $2N$ that

$$\langle \delta_0, R(A_F^{[N]})\delta_0 \rangle = \langle \delta_0, R(A)\delta_0 \rangle.$$

But this is false for $R(x) = x^2 P_{N-1}(x)^2$ since

$$\langle \delta_0, R(A)\delta_0 \rangle = \|A\delta_{N-1}\|^2 = a_{N-1}^2 + a_{N-2}^2 + b_{N-1}^2,$$

while

$$\langle \delta_0, R(A_F^{[N]})\delta_0 \rangle = \|A_N^{[F]}\delta_{N-1}\|^2 = a_{N-2}^2 + b_{N-1}^2.$$

Proof of Theorem 6. By (5.33) and (5.34) as $z \to 0$,

$$-\frac{Q_N(-\frac{1}{z})}{zP_N(-\frac{1}{z})} = \sum_{j=0}^{2N-1} \kappa_j z^j + O(z^{2N}). \tag{5.40}$$

Now $z^{N-1}Q_N(-\frac{1}{z})$ is a polynomial of degree $N-1$ since $Q_N(0) \neq 0$ and $z^N P_N(-\frac{1}{z})$ is a polynomial of degree N since $P_N(0) \neq 0$. Moreover, $\lim_{z\to 0} z^N P_N(-\frac{1}{z}) \neq 0$ since P_N has degree N. Thus (5.40) identifies $f^{[N-1,N]}$ and $-z^{N-1}Q_N(-\frac{1}{z})/z^N P_N(-\frac{1}{z})$. Similarly, noting that since $M_N(0) = 0$ (but $M_N'(0) \neq 0$ since A_K^N has simple eigenvalues), $z^N M_N(-\frac{1}{z})$ is a polynomial of degree $N-1$, and we identify $f^{[N-1,N-1]}(z)$ and $-z^{N-1}N_N(-\frac{1}{z})/z^N M_N(-\frac{1}{z})$. Theorem 5.2 thus implies Theorem 6. $\square$

Remarks. 1. Since P_N and Q_N are relatively prime (by Proposition 5.7) and similarly for M_N, N_N, we are in the situation where the numerator and denominator are uniquely determined up to a constant.

2. Suppose $\gamma_n \leq Ca^n$ so ρ is unique and supported on some interval $[0, R]$. Then if R is chosen as small as possible, $\sum_{n=0}^\infty \kappa_n z^n$ has radius of convergence R^{-1}, but the Padé approximants converge in the entire region $\mathbb{C}\backslash(-\infty, -R^{-1}]$!

Before leaving our discussion of Padé approximants for series of Stieltjes, we will consider the sequences $f^{[N+j,N]}(z)$ for j fixed. We will show they each converge as $N \to \infty$ with limits that are all distinct (as j varies) if the Stieltjes moment problem is indeterminate and all the same if a certain set of Stieltjes moment problems are all determinate.

Given a set of moments $\{\gamma_j\}_{j=1}^\infty$ and $\ell = 1, 2, \dots$, define for $j = 0, 1, \dots$

$$\gamma_j^{(\ell)} \equiv \frac{\gamma_{j+\ell}}{\gamma_\ell}. \tag{5.41}$$

Proposition 5.12. *Suppose that $\{\gamma_j\}_{j=0}^\infty$ is a set of Stieltjes (resp. Hamburger) moments. Then $\{\gamma_j^{(\ell)}\}_{j=0}^\infty$ is the set of moments for a Stieltjes (resp. Hamburger) problem for $\ell = 1, 2, \dots$ (resp. $\ell = 2, 4, 6, \dots$). This problem is indeterminate if the original problem is.*

Proof. We will consider the Stieltjes case. Let $\rho \in \mathcal{M}^S(\gamma)$. Then $\gamma_\ell^{-1} x^\ell \, d\rho(x) \equiv d\rho^{(\ell)}(x)$ solves the moment problem for $\gamma^{(\ell)}$. If $\rho_1, \rho_2 \in \mathcal{M}^S(\gamma)$, then $\rho_1^{(\ell)}, \rho_2^{(\ell)}$ are both in $\mathcal{M}^S(\gamma^{(\ell)})$. If $\rho_1^{(\ell)} = \rho_2^{(\ell)}$, then $\rho_1 - \rho_2$ is supported at zero, which means it is zero since $\int d\rho_1(x) = \gamma_0 = \int d\rho_2(x)$. Thus, if the γ problem is indeterminate, so is the $\gamma^{(\ell)}$ problem. $\square$

Example. As Corollary 4.21 shows, there can be determinate moment problems so that $\gamma^{(1)}$ is indeterminate (in the language of that corollary, $\tilde{\gamma}^{(1)} = \gamma$). Thus, the converse of the last statement in Proposition 5.12 fails.

As an aside, we present a proof of a criterion for indeterminacy of Hamburger [8], especially interesting because of a way of rewriting it in terms of a single ratio of determinants (see Theorem A.7). Note this aside deals with the Hamburger problem.

Proposition 5.13. *A necessary and sufficient condition for a set of Hamburger moments to be indeterminate is that*

(i) $\sum_{j=0}^\infty |P_j(0)|^2 < \infty$ *and*

(ii) $\sum_{j=0}^\infty |P_j^{(2)}(0)|^2 < \infty$

where $P_j^{(2)}(x)$ are the orthogonal polynomials for the $\gamma^{(2)}$ moment problem.

Proof. If $\{\gamma_j\}_{j=0}^\infty$ is indeterminate by Proposition 5.12, so is $\{\gamma_j^{(2)}\}_{j=0}^\infty$, and then (i), (ii) follow by Theorem 3. The converse is more involved. The intuition is the following: If $d\rho$ is an even measure, then $P_{2j}^{(2)}(x) = \sqrt{\gamma_2}\frac{P_{2j+1}(x)}{x}$, so $P_m^{(2)}(0) = \sqrt{\gamma_2}\frac{\partial P_{m+1}}{\partial x}(0)$ (both sides are zero if m is odd). So (ii) is equivalent to $\sum_{j=0}^\infty |\frac{\partial P_j(0)}{\partial x}|^2 < \infty$ and condition (v) of Theorem 3 says that (i), (ii) imply indeterminacy. Our goal is to prove in general that when (i) holds, $P_j^{(2)}(0)$ and $\frac{\partial P_{j+1}}{\partial x}(0)$ are essentially equivalent.

Let $S_n(x) = P_n^{(2)}(x)$, $\eta_n = \frac{\partial P_n}{\partial x}(0)$, and define

$$\alpha_n = \int x S_n(x) \, d\rho(x) \tag{5.42}$$

$$\beta_n = \int [x S_n(x)][P_{n+1}(x)] \, d\rho(x), \tag{5.43}$$

where ρ is any solution of the γ moment problem. Since S_n is an orthogonal polynomial for $d\rho^{(2)}$, we have

$$\int [x S_n(x)] x^j \, x d\rho(x) = 0, \qquad j = 0, 1, \dots, n-1$$

and thus

$$\int xS_n(x)P_j(x)\,d\rho(x) = \alpha_n P_j(0), \qquad j = 0, 1, \dots, n$$

so the orthogonal expansion for $xS_n(x)$ is

$$xS_n(x) = \beta_n P_{n+1}(x) + \alpha_n \sum_{j=0}^{n} P_j(0)P_j(x). \tag{5.44}$$

Since $xS_n(x)$ vanishes at zero,

$$\beta_n P_{n+1}(0) + \alpha_n \sum_{j=0}^{n} |P_j(0)|^2 = 0. \tag{5.45}$$

Since

$$\int |xS_n(x)|^2\,d\rho(x) = \gamma_2 \int S_n(x)^2\,d\rho^{(2)}(x) = \gamma_2,$$

we have by (5.44) that

$$\gamma_2 = \beta_n^2 + \alpha_n^2 \sum_{j=0}^{n} |P_j(0)|^2. \tag{5.46}$$

Moreover, taking derivatives of (5.44) at $x = 0$,

$$S_n(0) = \beta_n \eta_{n+1} + \alpha_n \sum_{j=0}^{n} P_j(0)\eta_j. \tag{5.47}$$

By (5.46), β_n is bounded, so by (5.45),

$$|\alpha_n| \le C_1 |P_{n+1}(0)|. \tag{5.48}$$

By hypothesis, $\sum_{j=0}^{\infty} |P_j(0)|^2 < \infty$, so $P_{n+1}(0) \to 0$ and thus by (5.46), $\beta_n \to \sqrt{\gamma_2}$ as $n \to \infty$. Since $\beta_n > 0$ for all n (this follows from the fact that both $xS_n(x)$ and $P_{n+1}(x)$ have positive leading coefficient multiplying x^{n+1}), we see that β_n^{-1} is bounded. Using (5.48), the Schwarz inequality on the sum in (5.47), and $\sum_{j=0}^{\infty} |P_j(0)|^2 < \infty$ again, we see that

$$\begin{aligned} |\eta_{n+1}|^2 &\le C\biggl(|S_n(0)|^2 + |P_{n+1}(0)|^2 \sum_{j=0}^{n} |\eta_j|^2\biggr) \\ &\le C(|S_n(0)|^2 + |P_{n+1}(0)|^2)\biggl(1 + \sum_{j=0}^{n} |\eta_j|^2\biggr). \end{aligned}$$

It follows that

$$\left[1+\sum_{j=0}^{n+1}|\eta_j|^2\right] \leq [1+C(|S_n(0)|^2+|P_{n+1}(0)|^2)]\left[1+\sum_{j=0}^{n}|\eta_j|^2\right]$$

and so by induction that

$$\sup_{1\leq n<\infty}\sum_{j=0}^{n+1}|\eta_j|^2 \leq \sup_{1\leq n<\infty}\prod_{j=1}^{n+1}[1+C(|S_{j-1}(0)|^2+|P_j(0)|^2)] < \infty$$

since $\sum_{j=0}^\infty |P_j(0)|^2 + \sum_{j=0}^\infty |S_j(0)|^2 < \infty$ by hypothesis. Thus, if (i) and (ii) hold, $\eta_n \in \ell_2$ and thus, the problem is indeterminate by Theorem 3. $\square$

Theorem 5.14. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Stieltjes moments. Fix $\ell \geq 1$ and let $P_N^{(\ell)}(z)$, $Q_N^{(\ell)}(z)$, $M_N^{(\ell)}(z)$, and $N_N^{(\ell)}(z)$ be the orthogonal polynomials and other associated polynomials for the $\gamma^{(\ell)}$ moment problem. Let $f^{[N,M]}(z)$ be the Padé approximants for the series of Stieltjes $\sum_{j=0}^\infty \kappa_j z^j$ where $\kappa_j = (-1)^j\gamma_j$. Then*

$$f^{[N+\ell-1,N]}(z) = \sum_{j=0}^{\ell-1}(-1)^j\gamma_j z^j + (-1)^\ell\gamma_\ell z^\ell\left[\frac{Q_N^{(\ell)}(-\frac{1}{z})}{zP_N^{(\ell)}(-\frac{1}{z})}\right] \tag{5.49}$$

and

$$f^{[N+\ell-1,N-1]}(z) = \sum_{j=0}^{\ell-1}(-1)^j\gamma_j z^j + (-1)^\ell\gamma_\ell z^\ell\left[\frac{N_N^{(\ell)}(-\frac{1}{z})}{zM_N^{(\ell)}(-\frac{1}{z})}\right]. \tag{5.50}$$

In particular:

1. *For each ℓ, $(-1)^\ell f^{[N+\ell-1,N]}(x)$ is monotone increasing to a finite limit for all $x \in (0,\infty)$.*
2. *For all $z \in \mathbb{C}\backslash(-\infty,0]$, $\lim_{N\to\infty} f^{[N+\ell-1,N]}(z) \equiv f_\ell(z)$ exists.*
3. *The $\gamma^{(\ell)}$ moment problem is (Stieltjes) determinate if and only if $f_\ell(z) = f_{\ell+1}(z)$.*
4. *If the $\gamma^{(\ell)}$ moment problem is determinate, then $f_0(z) = f_1(z) = \cdots = f_{\ell+1}(z)$.*
5. *If the $\gamma^{(\ell)}$ moment problem is indeterminate, then as $x \to \infty$,*

$$f_{\ell+1}(x) = (-1)^\ell\gamma_\ell\mu_K^{(\ell)}(\{0\})x^\ell + O(x^{\ell-1}), \tag{5.51}$$

where $\mu_K^{(\ell)}$ is the Krein solution of the $\gamma^{(\ell)}$ problem. In particular if $\ell > 1$, $-f_{\ell+1}(x)$ is not a Herglotz function (as it is if the problem is determinate).

Remarks. 1. Thus, it can happen (e.g., if γ is determinate but $\gamma^{(1)}$ is not (cf. Corollary 4.21) that $f^{[N-1,N]}$ and $f^{[N,N]}$ have the same limit, but that $f^{[N+1,N]}$ has a different limit.

2. If the $\{\gamma_j\}_{j=0}^\infty$ obey a condition that implies uniqueness and which is invariant under $\gamma_j \to \gamma_{j+1}$ (e.g., the condition of (1.12b) of Proposition 1.5), then all $\gamma^{(\ell)}$ are determinate; see Theorem 5.19 below.

3. Even for $\ell = 1$ and consideration of $f^{[N-1,N]}$ and $f^{[N,N]}$, we have something new — the remarkable fact that $x\,d\mu_K(x)/\gamma_1^{-1}$ is $d\mu_F^{(1)}(x)$. Multiplication by x kills the point measure at $x = 0$ and produces a measure supported on some set $[R, \infty)$ with $R > 0$. We also see that monotonicity for f_N^- implies monotonicity of f_N^+. The direction of monotonicity flips because of the minus sign ($(-1)^\ell = -1$) in (5.49).

4. In particular, we have $P_N^{(1)}(x) = c_N x^{-1} M_{N+1}(x)$, that is, for any $\ell \neq m$, $\int x^{-1} M_m(x) M_\ell(x)\, d\rho(x) = 0$, something that can be checked directly.

5. This theorem implies that all the $f^{[N,M]}$ with $N \geq M - 1$ exist and their denominators obey a three-term recursion relation.

6. The connection in Remark 3 extended to $x\,d\mu_K^{(\ell)}(x) = c_\ell\, d\mu_F^{(\ell+1)}(x)$ implies that if any $\gamma^{(\ell)}$ is indeterminate, then $d\mu_K(x)$ is a point measure. Thus if $\kappa_n = (-1)^n \int_0^\infty x^n\, d\rho(x)$ where ρ is associated to a determinate Stieltjes problem and $d\rho$ is not a point measure, then all the $f_\ell(z)$'s, $\ell = 0, 1, 2, \dots$, are equal.

Proof. It is easy to check that the right side of (5.49) and (5.50) are ratios of polynomials whose degrees are at most of the right size. (Because $P_N^{(\ell)}(0) \neq 0 \neq M_N^{(\ell)'}(0)$, it is easy that the denominators are always precisely of the right size.) Since $M_N^{(\ell)}(z)$ and $P_N^{(\ell)}(z)$ are of degree n, the rationalized denominators do not vanish at $\frac{1}{z} = 0$. By Proposition 5.11 for the $\gamma^{(\ell)}$ problem, they have the proper asymptotic series to be $f^{[N+\ell-1,N]}(z)$ and $f^{[N+\ell-1,N-1]}(z)$, respectively. That proves (5.49) and (5.50).

Assertions (1), (2), (3) are then just Theorem 6 for the $\gamma^{(\ell)}$ moments. To prove assertion (4), note that if $\gamma^{(\ell)}$ is determined by Proposition 5.12, so are $\gamma^{(\ell-1)}, \gamma^{(\ell-2)}, \dots, \gamma^{(1)}$, γ, and so by (3), we have $f_{\ell+1} = f_\ell = \cdots = f_0$.

To prove assertion (5), note that if the $\gamma^{(\ell)}$ moment problem is indeterminate, $d\mu_K^{(\ell)}(\{0\}) > 0$. Thus,

$$\lim_{x\to\infty} \int \frac{d\mu_K^{(\ell)}(y)}{1+xy} = \mu_K^{(\ell)}\{0\} > 0. \tag{5.52}$$

By (5.50),

$$f_{\ell+1}(x) = \sum_{j=0}^{\ell-1} (-1)^j \gamma_j x^j + (-1)^\ell \gamma_\ell x^\ell \int_0^\infty \frac{d\mu_K^{(\ell)}(y)}{1+xy}\,,$$

so (5.52) implies (5.51). □

To deal with the sequences $f^{[N-1+\ell,N]}(z)$ with $\ell < 0$, we need to introduce yet another modified moment problem associated to a set of Hamburger (or Stieltjes) moments. To motivate what we are looking for, let $\rho \in \mathcal{M}^H(\gamma)$ and let $G_\rho(z)$ be the associated Stieltjes transform. Then $-G_\rho(z)^{-1}$ is a Herglotz function which has an asymptotic series to all orders as $z \to i\infty$. Since $G_\rho(z) \sim -\frac{1}{z}(1 + \gamma_1 z^{-1} + \gamma_2 z^{-2} + O(z^{-3}))$,

$$-G_\rho(z)^{-1} \sim z - \gamma_1 - (\gamma_2 - \gamma_1^2) z^{-1} + O(z^{-2})$$

so (by the proof of Proposition 4.13) the Herglotz representation of $-G_\rho(z)^{-1}$ has the form

$$-G_\rho(z)^{-1} = z - \gamma_1 + (\gamma_2 - \gamma_1^2) \int \frac{d\tilde{\rho}(x)}{x - z}\,, \tag{5.53}$$

where $d\tilde{\rho}$ is a normalized measure. Its moments, which we will call $\gamma_j^{(0)}$, only depend on the asymptotic series for $G_\rho(z)$, and so only on the original moments. We could do everything abstractly using (5.53), but we will be able to explicitly describe the relation between the moment problems.

The key is the following formula, a Ricatti-type equation well known to practitioners of the inverse problem [6] (which we will, in essence, prove below):

$$-m_0(z)^{-1} = z - b_0 + a_0^2 m_1(z), \tag{5.54}$$

where $m_0(z) = \langle \delta_0, (A - z)^{-1}\delta_0\rangle$ is just $G_\rho(z)$ for a spectral measure, and $m_1(z) = \langle \delta_0, (A^{[1]} - z)^{-1}\delta_0\rangle$, where $A^{[1]}$ is obtained from A by removing the top row and left-most column. (5.54) is just (5.53) if we note that $b_0 = \gamma_1$ and $a_0^2 = \gamma_2 - \gamma_1^2$. Thus, we are led to define $\gamma_j^{(0)}$ as the moments associated to the Jacobi matrix $A^{[1]}$ obtained by removing the top row and left-most column, that is,

$$A^{[1]} = \begin{pmatrix} b_1 & a_1 & 0 & \dots & \dots \\ a_1 & b_2 & a_2 & \dots & \dots \\ 0 & a_2 & b_3 & a_3 & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots \end{pmatrix}.$$

Proposition 5.15. *Let $\{\gamma_j\}_{j=0}^\infty$ be a set of Hamburger moments. Then the $\{\gamma_j^{(0)}\}_{j=0}^\infty$ Hamburger problem is determinate if and only if $\{\gamma_j\}_{j=0}^\infty$ is.*

Proof. Let $\tilde{A}^{[1]}$ be $A^{[1]}$ with a row of zeros added at the top and column of zeros on the left. Since $\tilde{A}^{[1]} = 0 \oplus A^{[1]}$, $\tilde{A}^{[1]}$ is essentially self-adjoint if and only if $A^{[1]}$ is. $A - \tilde{A}^{[1]}$ is a matrix with three non-zero elements and essential self-adjointness is provided by bounded perturbations. Thus, A is essentially self-adjoint if and only if $A^{[1]}$ is. By Theorem 2, we have the equivalence of determinacy for the Hamburger problem. □

Remark. As we will see shortly, this result is not true in the Stieltjes case.

Let $P_N^{(0)}(x)$, $Q_N^{(0)}(x)$, and $f_N^{(0)}(z) = -\frac{Q_N^{(0)}(z)}{P_N^{(0)}(z)}$ be the polynomials and finite matrix approximation for the $\gamma^{(0)}$ problem. Then

Proposition 5.16.

$$\text{(i)} \qquad P_N^{(0)}(x) = a_0 Q_{N+1}(x) \tag{5.56}$$

$$\text{(ii)} \qquad Q_N^{(0)}(x) = -\frac{1}{a_0}\, P_{N+1}(x) + \frac{x - b_0}{a_0}\, Q_{N+1}(x) \tag{5.57}$$

$$\text{(iii)} \qquad -f_{N+1}^{-}(z)^{-1} = z - b_0 + a_0^2 f_N^{(0)}(z) \tag{5.58}$$

Remarks. 1. (i) implies that the Q_N's are orthogonal polynomials for some measure.

2. (5.58) is (5.54).

Proof. For each fixed x, $P_N^{(0)}(x), Q_N^{(0)}(x)$ obey the same difference equation as $P_{N+1}(x)$, $Q_{N+1}(x)$ so we need (5.56), (5.57) at the initial points $N=-1,0$ where it is required that

$$P_{-1}^{(0)}(x)=0, \quad P_0^{(0)}(x)=1; \qquad Q_{-1}^{(0)}(x)=-\frac{1}{a_0}, \quad Q_0^{(0)}(x)=0$$

($Q_{-1}^{(0)}(x) = -\frac{1}{a_0}$ since we don't make the convention $a_{-1}^{(0)}=1$, but rather $a_{-1}^{(0)}=a_0$ consistent with $a_n^{(0)}=a_{n+1}$). This is consistent with (5.56) if we note that

$$Q_0(x)=0, \quad Q_1(x)=\frac{1}{a_0}; \qquad P_0(x)=1, \quad P_1(x)=\frac{(x-b_0)}{a_0}\,.$$

This proves (i), (ii).

They in turn imply

$$a_0^2\,\frac{Q_N^{(0)}(x)}{P_N^{(0)}(x)} = x-b_0-\frac{P_{N+1}(x)}{Q_{N+1}(x)}\,,$$

which, by (5.12), proves (iii). □

Proposition 5.17. *Let $\{\gamma_j\}_{j=0}^\infty$ be a set of Stieltjes moments. If the Hamburger problem is indeterminate, then the $\gamma^{(0)}$ Stieltjes problem is indeterminate (even if the γ Stieltjes problem is determinate).*

Proof. As we will see below (Proposition 5.22 $\equiv$ Theorem 8), a set of Stieltjes moments which is Hamburger indeterminate is Stieltjes determinate if and only if $L \equiv \lim_{N\to\infty}[-\frac{Q_N(0)}{P_N(0)}]$ is infinite. By (5.58),

$$a_0^2 L^{(0)} = b_0 - L^{-1}.$$

Since $L>0$, $L^{(0)}$ is never infinite. □

Remarks. 1. Thus, if γ is Hamburger indeterminate but Stieltjes determinate, γ and $\gamma^{(0)}$ have opposite Stieltjes determinacy.

2. The spectral way to understand this result is to note that if γ is Hamburger indeterminate, the Friedrichs extensions of A and $A^{[1]}$ have interlacing eigenvalues. Given that $A\geq 0$, $A^{[1]}$ must be strictly positive.

For $\ell<0$ and integral, we let

$$\gamma_j^{(\ell)} = [\gamma^{(0)}]_j^{(-\ell)} = \frac{\gamma_{j-\ell}^{(0)}}{\gamma_{-\ell}^{(0)}}\,.$$

Then:

Theorem 5.18. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Stieltjes moments. Fix $\ell \le 0$ and let $P_N^{(\ell)}(z)$, $Q_N^{(\ell)}(z)$, $M_N^{(\ell)}(z)$, and $N_N^{(\ell)}(z)$ be the orthogonal polynomials and other associated polynomials for the $\gamma^{(\ell)}$ moment problem. Let $f^{[N,M]}(z)$ be the Padé aproximants for the series of Stieltjes $\sum_{j=0}^\infty \kappa_j z^j$ where $\kappa_j = (-1)^j\gamma_j$. Then*

$$f^{[N+\ell-1,N]}(z) = \left\{1-\gamma_1 z - \sum_{j=0}^{-\ell-1} (-1)^j \gamma_j^{(0)} z^{j+2} + (-1)^{\ell+1}\gamma_{-\ell}^{(0)} z^{-\ell+2}\left[\frac{Q_{N+\ell-1}^{(\ell)}(-\frac{1}{z})}{zP_{N+\ell-1}^{(\ell)}(-\frac{1}{z})}\right]\right\}^{-1} \tag{5.59}$$

and

$$f^{[N+\ell-1,N+1]}(z) = \left\{1-\gamma_1 z - \sum_{j=0}^{-\ell-1} (-1)^j \gamma_j^{(0)} z^{j+2} + (-1)^{\ell+1}\gamma_{-\ell}^{(0)} z^{-\ell+2}\left[\frac{N_{N+\ell-1}^{(\ell)}(-\frac{1}{z})}{zM_{N+\ell}^{(\ell)}(-\frac{1}{z})}\right]\right\}^{-1}. \tag{5.60}$$

In particular,

(1) *For each ℓ, $(-1)^\ell f^{[N+\ell-1,N]}(x)$ is monotone increasing to a finite limit for all $x\in(0,\infty)$.*
(2) *For all $z\in\mathbb{C}\backslash(-\infty,0]$, $\lim_{N\to\infty} f^{[N+\ell-1,N]}(z) \equiv f_\ell(z)$ exists.*
(3) *The $\gamma^{(\ell)}$ moment problem is Stieltjes determinate if and only if $f_\ell(z) = f_{\ell-1}(z)$.*
(4) *If the $\gamma^{(\ell)}$ moment problem is determinate, then $f_0(z) = f_{-1}(z) = \cdots = f_\ell(z) = f_{\ell-1}(z)$.*
(5) *If the $\gamma^{(\ell)}$ moment problem is indeterminate, then as $x\to\infty$,*

$$f_{\ell-1}(x) = (-1)^{\ell+1}(\gamma_{-\ell}^{(0)})^{-1} x^{\ell-2}\mu_K^{(\ell)}(\{0\})^{-1} + O(x^{\ell-3}),$$

where $\mu_K^{(\ell)}$ is the Krein solution of the $\gamma^{(\ell)}$ problem. In particular, $-f_{\ell-1}(x)$ is not a Herglotz function (as it is if the problem is determinate).

Proof. By (5.58), we have a relation between formal power series:

$$\left(\sum_{j=0}^\infty (-1)^j\gamma_j z^j\right)^{-1} = 1+\gamma_1 z - (\gamma_2-\gamma_1^2)z^2\left[\sum_{j=0}^\infty (-1)^j \gamma_j^{(0)} z^j\right], \tag{5.61}$$

from which one obtains

$$f^{[M,N+2]}(z) = (1+\gamma_1 z - (\gamma_2-\gamma_1^2)z^2 f^{(0)[N,M]}(z))^{-1}.$$

Thus, (5.59) is just (5.49) and (5.60) is (5.50). The consequence (1)–(5) follows as in the proof of Theorem 5.14. $\square$

We summarize and extend in the following:

Theorem 5.19. *Let $\sum_{j=0}^{\infty} \kappa_j z^j$ be a series of Stieltjes. Then for each $\ell = 0, \pm 1, \pm 2, \dots$, $f_\ell(z) = \lim_{N\to\infty} f^{[N+\ell,N]}(z)$ exists uniformly for z in compact subsets of $\mathbb{C}\backslash(-\infty,0]$. Moreover,*

1. *If any two f_ℓ's are different, then all of them are meromorphic.*
2. *If the $|\kappa_j| = \gamma_j$ moment problem is determinate and the measure solving the moment problem is not a discrete point measure, then all f_ℓ's are equal.*
3. *If $|\kappa_j| \le C^j (2j)!$, then all f_ℓ's are equal.*

Proof. The first assertion is Theorem 5.14 for $\ell \ge 1$ and Theorem 5.18 for $\ell \le 0$. If some $f_\ell \ne f_{\ell+1}$, then some $\gamma^{(\ell)}$ are indeterminate, so the corresponding $d\rho_F$'s are pure point and f_ℓ's meromorphic. This proves (1). Under the hypothesis of (2), f_0 is not meromorphic, so by (1), all f's are equal. To prove (3), an induction using (5.61) proves $|\gamma_j^{(0)}| \le \tilde{C}^j (2j)!$, so by Proposition 1.5, all the $\gamma^{(\ell)}$ moment problems are determinate. $\square$

This completes our discusion of Padé approximants for series of Stieltjes. We return to consequences of Theorem 5.2 for the study of the Stieltjes moment problem.

As we have seen for any $x > 0$, $-\frac{Q_N(-x)}{P_N(-x)}$ is monotone increasing and $-\frac{xN_N(-x)}{M_N(-x)}$ is monotone decreasing. By taking limits (recall $M_N(0) = 0$), we see that $-\frac{Q_N(0)}{P_N(0)}$ is monotone increasing and $\frac{N_N(0)}{M_N'(0)}$ is decreasing.

Proposition 5.20.

$$\text{(i)} \qquad \lim_{N\to\infty} -\frac{Q_N(0)}{P_N(0)} = \int y^{-1}\, d\mu_F(y)$$

$$\text{(ii)} \qquad \lim_{N\to\infty} \frac{N_N(0)}{M_N'(0)} = \mu_K(\{0\}),$$

where μ_F (resp. μ_K) is the Friedrichs (resp. Krein) solution.

Proof. By Theorem 5.2 and Proposition 5.6, for $x > 0$,

$$-\frac{Q_N(-x)}{P_N(-x)} \le \int (y+x)^{-1}\, d\mu_F(y),$$

so taking x to zero and N to infinity, we see that

$$\lim_{N\to\infty} -\frac{Q_N(0)}{P_N(0)} \le \int y^{-1}\, d\mu_F(y).$$

On the other hand, since $-\frac{Q_N(-x)}{P_N(-x)} = (\delta_0, (A_F^{[N]} + x)^{-1}\delta_0)$ is monotone increasing as x decreases, we have for each N and $x > 0$,

$$-\frac{Q_N(-x)}{P_N(-x)} \le \lim_{N\to\infty} -\frac{Q_N(0)}{P_N(0)}\,,$$

so taking N to infinity for fixed $x > 0$ and using Theorem 5.2,

$$\int (x+y)^{-1}\, d\mu_F(y) \le \lim_{N\to\infty} -\frac{Q_N(0)}{P_N(0)}\,.$$

Taking x to zero, we see that

$$\int y^{-1}\, d\mu_F(y) \le \lim_{N\to\infty} -\frac{Q_N(0)}{P_N(0)}\,,$$

so (i) is proven.

The proof of (ii) is similar. By Theorem 5.2 and Proposition 5.8,

$$-\frac{xN_N(-x)}{M_N(-x)} \ge \int \frac{x}{y+x}\, d\mu_K(y) \ge \mu_K(\{0\}),$$

so taking x to zero and N to infinity,

$$\lim_{N\to\infty} \frac{N_N(0)}{M_N'(0)} \ge \mu_K(\{0\}).$$

On the other hand, since $-\frac{xN_N(-x)}{M_N(-x)} = (\delta_0, x(A_K^{[N]}+x)^{-1}\delta_0)$ is monotone decreasing as x decreases, we have for each N and $x > 0$,

$$-\frac{xN_N(-x)}{M_N(-x)} \ge \lim_{N\to\infty} \frac{N_N(0)}{M_N'(0)}\,,$$

so taking N to infinity for fixed $x > 0$ and using Theorem 5.2,

$$\int \frac{x}{x+y}\, d\mu_K(y) \ge \lim_{N\to\infty} \frac{N_N(0)}{M_N'(0)}\,.$$

Taking x to zero, we see that

$$\mu_K(\{0\}) \ge \lim_{N\to\infty} \frac{N_N(0)}{M_N'(0)}\,,$$

so (ii) is proven. $\square$

This leads us to define (note that we use $\frac{M_N'(0)}{N_N(0)}$, not $\frac{N_N(0)}{M_N'(0)}$ so $M, L \in (0,\infty)\cup\{\infty\}$):

$$L = \lim_{N\to\infty} -\frac{Q_N(0)}{P_N(0)} \tag{5.62}$$

$$M = \lim_{N\to\infty} \frac{M_N'(0)}{N_N(0)}, \tag{5.63}$$

so Proposition 5.20 says that

$$L = \int y^{-1}\, d\mu_F(y)$$
$$M^{-1} = \mu_K(\{0\}).$$

By (4.25), $\mu_K(\{0\}) = 1/\sum_{n=0}^\infty |P_N(0)|^2$, so

$$M = \sum_{n=0}^\infty |P_n(0)|^2. \tag{5.64}$$

Note. (4.25) was only proven in the indeterminate case, but the argument applies in the determinate case also. If x is an eigenvalue of a solution μ of the moment problem associated to a self-adjoint extension, then $\mu(\{x\}) = 1/\sum_{n=0}^\infty |P_n(x)|^2$.

Theorem 5.21 ($\equiv$ Theorem 7). *Let $\{\gamma_n\}_{n=0}^\infty$ be the moments of a Stieltjes problem. Then the problem is indeterminate if and only if*

$$L < \infty \qquad \text{and} \qquad M < \infty.$$

Equivalently, the problem is determinate if and only if

$$L = \infty \qquad \text{or} \qquad M = \infty.$$

Proof. If $L < \infty$ and $M < \infty$, then $\int y^{-1} d\mu_F(y) < \infty$, while $\mu_K(\{0\}) > 0$, so clearly, $\mu_F \neq \mu_K$ and the problem is indeterminate. Conversely, if the problem is indeterminate, then by Proposition 3.1, $\alpha = \inf \operatorname{spec}(A_F) > 0$, so $\int y^{-1}\, d\mu_F(y) \leq \alpha^{-1} < \infty$ and $L < \infty$. Moreover, since the Stieltjes problem is indeterminate, so is the Hamburger problem; and thus by (5.64), $M < \infty$. $\square$

Theorem 5.22 ($\equiv$ Theorem 8). *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Stieltjes moments. Then the Stieltjes problem is determinate while the Hamburger problem is indeterminate if and only if*

$$\sum_{n=0}^\infty |Q_n(0)|^2 < \infty \tag{5.65}$$

and $L = \infty$.

Proof. For a set of Stieltjes moments $-\frac{Q_n(0)}{P_n(0)}$ is positive and monotone increasing, so $|Q_n(0)| \geq \frac{|Q_1(0)P_n(0)|}{|P_1(0)|}$. Since $Q_1(0) \neq 0$, we see that (5.65) implies also that $M < \infty$. Thus, (5.65) is equivalent to the Hamburger problem being indeterminate. Given that $M < \infty$, Theorem 5.21 says that determinacy of the Stieltjes problem is equivalent to $L = \infty$. $\square$

As our next topic, we will further examine the conditions $M < \infty$ and $L < \infty$ to see they are conditions of Stieltjes and Krein in a different form. Define

$$\ell_n = -\frac{Q_n(0)}{P_n(0)} + \frac{Q_{n-1}(0)}{P_{n-1}(0)}\,, \qquad n \geq 1 \tag{5.66}$$

and

$$m_n = \frac{M_n'(0)}{N_n(0)} - \frac{M_{n-1}'(0)}{N_{n-1}(0)}\,, \qquad n \geq 2 \tag{5.67a}$$

$$m_1 = \frac{M_1'(0)}{N_1(0)}\,. \tag{5.67b}$$

By the monotonicity properties of this section, $\ell_n > 0$, $m_n > 0$. By definition and $Q_0(0) = 0$,

$$-\frac{Q_N(0)}{P_N(0)} = \sum_{n=1}^{N} \ell_n, \qquad L = \sum_{n=1}^{\infty} \ell_n$$

$$\frac{M_N'(0)}{N_N(0)} = \sum_{n=1}^{N} m_n, \qquad M = \sum_{n=1}^{\infty} m_n.$$

Proposition 5.23. *For $N \geq 1$,*

$$m_N = |P_{N-1}(0)|^2 \tag{5.68}$$

$$\ell_N = -[a_{N-1} P_N(0) P_{N-1}(0)]^{-1}. \tag{5.69}$$

Remark. Since $A_F^{[N]} > 0$, $P_N(z)$ has no zeros on $(-\infty, 0]$ and thus, $P_N(z)$ has the same sign near $-\infty$ and 0. But $P_N(z) = c_N z^N +$ lower order with $c_N > 0$, so $(-1)^N P_N(0) > 0$ (cf. (5.13)). Thus, $P_N(0)P_{N-1}(0) < 0$ and the minus sign in (5.69) is just what is needed to ensure that $\ell_N > 0$.

Proof. $A_K^{[N]}$ has $\{P_0(0), \dots, P_{N-1}(0)\}$ as its eigenfunction with eigenvalue zero. Thus, $\lim_{x\to 0} x(\delta_0, (A_K^{[N]} + x)^{-1}\delta_0) = |P_0(0)|^2 / \sum_{j=0}^{N-1} |P_j(0)|^2$. Since $P_0(0) = 1$, we see that

$$\frac{M_N'(0)}{N_N(0)} = \sum_{j=0}^{N-1} |P_j(0)|^2, \tag{5.70}$$

which implies (5.68). (5.69) follows immediately from Proposition 4.1. $\square$

Corollary 5.24. *If A given by* (1.16) *is the Jacobi matrix associated to an indeterminate Stieltjes moment problem, then*

$$\sum_{n=0}^{\infty} a_n^{-1/2} < \infty.$$

In particular, if $\sum_{n=0}^{\infty} a_n^{-1/2} = \infty$ for the Jacobi matrix associated to a Stieltjes problem, then the problem is determinate.

Proof. If the problem is indeterminate, by Proposition 5.23 and Theorem 5.21, $a_n^{-1/2}|P_n(0)P_{n-1}(0)|^{-1/2}$ and $|P_n(0)P_{n-1}(0)|^{1/2}$ both lie in ℓ^2, so their product lies in ℓ^1. $\square$

Now we will define, following Stieltjes and Krein, functions

$$U_n(x) = \frac{P_n(-x)}{P_n(0)}, \qquad n \geq 0 \tag{5.71}$$

$$V_n(x) = -\frac{Q_n(-x)}{P_n(0)}, \qquad n \geq 0 \tag{5.72}$$

$$G_n(x) = -a_{n-1} M_n(-x) P_{n-1}(0), \qquad n \geq 1 \tag{5.73}$$

$$H_n(x) = a_{n-1} N_n(-x) P_{n-1}(0), \qquad n \geq 1. \tag{5.74}$$

We claim that

Proposition 5.25.

(i) $U_n(0) = 1$
(ii) $G_n(0) = 0$
(iii) $H_n(0) = 1$
(iv) $U_n(x)H_n(x) - V_n(x)G_n(x) = 1$ for $n \geq 1$
(v) $f_n^+(-x) - f_n^-(-x) = \frac{1}{U_n(x)G_n(x)}$ for $n \geq 1$

Proof. (i) is immediate from the definition (5.71), (ii) from $M_n(0) = 0$, and (iii) follows from Proposition 4.1 and the definition (5.16) of N_N (and explains why we multiply M and N by $a_{n-1}P_{n-1}(0)$). To prove (iv), we note that for some constants $\alpha_n, \beta_n, \gamma_n$,

$$U_n(x) = \alpha_n P_n(-x), \qquad V_n(x) = -\alpha_n Q_n(-x)$$
$$G_n(x) = \beta_n P_n(-x) + \gamma_n P_{n-1}(-x), \qquad H_n(x) = -\beta_n Q_n(-x) - \gamma_n Q_{n-1}(-x),$$

so

$$U_n(x)H_n(x) - V_n(x)G_n(x) = -\alpha_n \gamma_n [P_n(-x)Q_{n-1}(-x) - Q_n(-x)P_{n-1}(-x)]$$

is constant as x is varied for fixed n. But at $x = 0$, by (i)–(iii) this combination is 1. (v) follows from (iv) and the definitions. $\square$

The following says that for $x > 0$, U, G can be associated with the equation of motion of a string of beads (see [1]). This is the starting point of deep work of Krein [17].

Theorem 5.26.
(i) $U_n(x) - U_{n-1}(x) = \ell_n G_n(x), \quad n \geq 1$
(ii) $G_{n+1}(x) - G_n(x) = m_{n+1} x U_n(x), \quad n \geq 1$
(iii) $G_1(x) = m_1 x \quad U_0(x) = 1$

Proof. (i) By definition of U_n,

$$U_n(x) - U_{n-1}(x) = \frac{M_n(-x)}{P_n(0)} = \ell_n G_n(x)$$

by (5.69) and (5.73).

(ii) We have for $n \geq 1$,

$$a_n P_{n+1}(-x) + b_n P_n(-x) + a_{n-1} P_{n-1}(-x) = -x P_n(-x). \tag{5.75}$$

(5.75) for $x = 0$ implies that

$$b_n = -a_n P_{n+1}(0) P_n(0)^{-1} - a_{n-1} P_{n-1}(0) P_n(0)^{-1}, \tag{5.76}$$

which we can substitute into (5.75) to obtain

$$a_n M_{n+1}(-x) - a_{n-1} P_{n-1}(0) P_n(0)^{-1} M_n(-x) = -x P_n(x).$$

Multiplying by $-P_n(0)$ and using the definitions (5.71)/(5.73), we see

$$G_{n+1}(x) - G_n(x) = x P_n(0)^2 U_n(x)$$

so (5.68) implies the result.

(iii) $U_0(x)$ is a constant so $U_0(0) = 1$ implies $U_0(x) \equiv 1$. G_1 is a linear polynomial with $G_1(0) = 0$, so $G_1(x) = G_1'(0)x$. For any n, $G_n'(0) = \lim_{x \downarrow 0} \frac{x^{-1} G_n(x)}{H_n(x)} = \sum_{j=1}^n m_j$. $\square$

We can use these equations to get further insight into Theorem 5.2. First, we obtain explicit bounds on the rate of convergence of $f_N^+(-x) - f_N^-(-x)$ to zero in the determinate case, where either $\sum m_j$ or $\sum \ell_j$ or both diverge.

Theorem 5.27. *For $x > 0$,*

$$f_N^+(-x) - f_N^-(-x) \leq \left[m_1 x^2 \left(\sum_{j=1}^n m_j \right) \left(\sum_{j=1}^n \ell_j \right) \right]^{-1}.$$

Proof. It follows from Theorem 5.26 and induction that $U_n(x)$ and $G_n(x)$ are non-negative for $x > 0$ and then that they are monotone in n. In particular, $U_n(x) \geq 1$, $G_n(x) \geq m_1 x$ from which, by (i), (ii),

$$U_n(x) \geq m_1 \left(\sum_{j=1}^n \ell_j \right) x$$

$$G_n(x) \geq \left(\sum_{j=1}^n m_j \right) x.$$

(v) of Proposition 5.25 then completes the proof. $\square$

And we obtain directly that in the indeterminate case, $f^\pm$ are meromorphic functions.

Theorem 5.28. (i) *For any $z \in \mathbb{C}$, we have that for $n \geq 1$,*

$$|U_n(z)| \leq \prod_{j=1}^{n}(1+\ell_j)\prod_{j=1}^{n}(1+m_j|z|)$$
$$|G_n(z)| \leq \prod_{j=1}^{n-1}(1+\ell_j)\prod_{j=1}^{n}(1+m_j|z|).$$

(ii) *If $M < \infty$ and $L < \infty$, then for all $z \in \mathbb{C}$, $U_n(z), V_n(z), G_n(z), H_n(z)$ converge to functions $U_\infty(z), V_\infty(z), G_\infty(z), H_\infty(z)$, which are entire functions obeying*

$$|f(z)| \leq C_\varepsilon \exp(\varepsilon(z))$$

for each $\varepsilon > 0$.
(iii) $f^-(z) = \frac{V_\infty(-z)}{U_\infty(-z)}$, $f^+(z) = \frac{H_\infty(-z)}{G_\infty(-z)}$.
(iv) $f^+(z) - f^-(x) = \frac{1}{U_\infty(-z)G_\infty(-z)}$.

Remark. In terms of the Nevanlinna functions A, B, C, D, one can see (using the fact that the Friedrichs solution is associated to B_t with $t = L$) that $G_\infty(-z) = -D(z)$, $H_\infty(-z) = C(z)$, $U_\infty(-z) = -B(z) - LD(z)$, and $V_\infty(-z) = A(z) + LC(z)$, where $L = \sum_{j=1}^\infty \ell_j$.

Proof. (i) follows by an elementary induction from Theorem 5.26. Similarly, one follows the proof of that theorem to show that V_n, H_n obey

$$\begin{aligned}
&V_n(x) - V_{n-1}(x) = \ell_n H_n(x), && n \geq 1\\
&H_{n+1}(x) - H_n(x) = m_{n+1} x V_n(x), && n \geq 1\\
&H_1(x) = 1 \qquad V_0(x) = 0
\end{aligned}$$

and obtains inductively that

$$|V_n(z)| \leq \prod_{j=1}^{n}(1+\ell_j)\prod_{j=2}^{n}(1+m_j|z|)$$
$$|H_n(z)| \leq \prod_{j=1}^{n-1}(1+\ell_j)\prod_{j=2}^{n}(1+m_j|z|).$$

Thus, if $L, M < \infty$, we first see that U, V, H, G are bounded and then, since $\sum_{j\geq n}\ell_j \to 0$, $\sum_{j\geq n} m_j \to 0$, that each sequence is Cauchy as $n \to \infty$. The C_ε bound is easy for products $\prod_{j=1}^\infty (1+m_j|z|)$ with $\sum_1^\infty m_j < \infty$. (iii), (iv) are then immediate from the definitions. $\square$

To make the link to Stieltjes' continued fractions, we need to note the relation between a_n, b_n, ℓ_n, and m_n. Immediately from Proposition 5.23, we have

$$a_n = \left(\ell_{n+1}\sqrt{m_{n+1}m_{n+2}}\,\right)^{-1}, \qquad n \geq 0 \tag{5.77}$$

and by (5.76),

$$b_n = m_{n+1}^{-1}(\ell_n^{-1} + \ell_{n+1}^{-1}), \qquad n \geq 1 \tag{5.78}$$

$$b_0 = m_1^{-1}\ell_1^{-1}. \tag{5.79}$$

(Parenthetically, we note that these equations can be used inductively to define m_j, ℓ_j given a_j, b_j. We have $m_1 = 1$, so (5.79) gives ℓ_1. Given $\ell_1, \dots, \ell_j$ and $m_1, \dots, m_j$, we can use a_{j-1} and (5.77) to find m_{j+1} and then b_j and (5.78) to get ℓ_{j+1}.)

Stieltjes' continued fractions are of the form (5.1b). Let

$$d_0 = c_1^{-1}, \qquad d_n = (c_n c_{n+1})^{-1} \tag{5.80}$$

for $n \geq 1$ so (5.1b) becomes

$$\cfrac{d_0}{w + \cfrac{d_1}{1 + \cfrac{d_2}{w + \dots}}}$$

Now use the identity

$$w + \cfrac{\beta_1}{1 + \cfrac{\beta_2}{f(w)}} = w + \beta_1 - \frac{\beta_1\beta_2}{\beta_2 + f(w)}$$

to see that (5.1b) has the form (5.1a) if $w = -z$, $d_0 = 1$, and

$$b_0 = d_1 \tag{5.81a}$$

$$b_n = d_{2n+1} + d_{2n} \tag{5.81b}$$

$$a_n^2 = d_{2n+1}d_{2n+2}. \tag{5.81c}$$

Thus, (5.80) and (5.81) are consistent with (5.77)–(5.79) if and only if

$$c_{2j-1} = m_j, \qquad c_{2j} = \ell_j. \tag{5.82}$$

Thus, we have seen that (5.1a) is (5.1b) if $w = -z$ and the c's are given by (5.82). Stieltjes' criterion that depends on whether or not $\sum_{j=1}^\infty c_j < \infty$ is equivalent to $L < \infty$ and $M < \infty$.

The connection (5.82) is not surprising. In (5.1b) if $w = 0$, the continued fraction formally reduces to $c_2 + c_4 + \cdots$ consistent with $\sum_{j=1}^\infty \ell_j = -\lim_{N\to\infty} \frac{Q_N(0)}{P_N(0)}$. On the other hand, if we multiply by w, the continued fraction formally becomes

$$\cfrac{1}{c_1 + \cfrac{1}{c_2 w + \cfrac{1}{c_3 + \cdots}}}$$

which, formally at $w = 0$, is $(c_1 + c_3 + \cdots)^{-1}$, consistent with $\sum_{j=1}^\infty m_j = \lim_{N\to\infty} \lim_{x\downarrow 0} [-\frac{xN_N(-x)}{M_N(-x)}]$.

We conclude this section by discussing Padé approximants for the Hamburger analog of series of Stieltjes. A series of Hamburger is a formal power series $\sum_{j=0}^\infty \kappa_j z^j$ with

$$\kappa_j = (-1)^j \int_{-\infty}^\infty x^j \, d\rho(x)$$

for some measure ρ. We will begin with the "principal" Padé approximants $f^{[N-1,N]}(z)$:

Theorem 5.29. *Let $\sum_{j=0}^\infty \kappa_j x^j$ be a series of Hamburger. Then:*

(i) *The $f^{[N-1,N]}(z)$ Padé approximants always exist and are given by*

$$f^{[N-1,N]}(z) = (\delta_0, (1 + zA_F^{[N]})^{-1}\delta_0) = -\frac{z^{N-1}Q_N(-\frac{1}{z})}{z^N P_N(\frac{1}{z})}\,. \tag{5.83}$$

(ii) *If the associated Hamburger moment problem is determinate, then for any z with $\operatorname{Im} z \neq 0$,*

$$\lim_{N\to\infty} f^{[N-1,N]}(z) = -\frac{z^{N-1}Q_N(-\frac{1}{z})}{z^N P_N(\frac{1}{z})} \tag{5.84}$$

exists and equals $\int \frac{d\rho(x)}{1+zx}$ for the unique solution, ρ, of the moment problem.

(iii) *The sequence $f^{[N-1,N]}(z)$ is pre-compact in the family of functions analytic in $\mathbb{C}_+$ (in the topology of uniform convergence on compact sets).*

(iv) *Any limit of $f^{[N-1,N]}(z)$ is of the form $\int \frac{d\rho(x)}{1+zx}$ where ρ is a von Neumann solution of the Hamburger problem.*

Proof. (i) The proof that (5.12) holds (Proposition 5.6) is the same as in the Stieltjes case, and from there we get (5.34) as in the Stieltjes case. Since $\lim_{z\to 0} z^N P_N(\frac{1}{z}) \neq 0$, we see $f^{[N-1,N]}(z)$ exists and is given by (5.83).

(iii) Since

$$|zf^{[N-1,N]}(z)| = |(\delta_0, (A_F^{[N]} + z^{-1})^{-1}\delta_0)| \leq |\operatorname{Im}(z^{-1})|^{-1},$$

we see that

$$|f^{[N-1,N]}(z)| \leq |z| \, |\mathrm{Im}(z)|^{-1}$$

is bounded on compacts. By the Weierstrass-Vitali theorem, such functions are precompact.

(ii), (iv) By the proof of Proposition 4.13, if $d\rho$ is any measure whose first $M+2$ moments are $\gamma_0, \gamma_1, \dots, \gamma_{M+2}$, then

$$\left| y^{M+1} \left[G_\rho(iy) + \sum_{n=0}^{M} (-i)^{n+1} y^{-n-1} \gamma_n \right] \right| \leq a y^{-1} \tag{5.85}$$

with a only depending on $\{\gamma\}$ (either $a = \gamma_{M+1}$ or $a = \frac{1}{2}[\gamma_M + \gamma_{M+2}]$). Since $\langle \delta_0, (A_F^{[N]})^j \delta_0 \rangle = \gamma_j$ for $j \leq 2N-1$, we see that for M fixed, (5.85) holds uniformly for N large if $G_N(z) = -z^{-1} f^{[N-1,N]}(-\frac{1}{z})$, so any limit point of the G's obeys (5.85) and is Herglotz. Thus by Proposition 4.13, it is of the form $G_\rho(z)$ with $\rho \in \mathcal{M}^H(\gamma)$. Thus the limit for $f^{[N-1,N]}(z)$ as $N \to \infty$, call it $f(z)$, has the form

$$f(z) = \int \frac{d\rho(x)}{1+xz}$$

with $\rho \in \mathcal{M}^H(\gamma)$. In the determinate case, ρ must be the unique solution, so all limit points are equal. Thus compactness implies convergence, and we have proven (ii).

In the indeterminate case, we note that $\delta_j = P_j(A_F^{[N]})\delta_0$ for $j = 0, \dots, N-1$ so

$$(A_F^{[N]} - z)^{-1} \delta_0 = \sum_{j=0}^{N-1} \langle P_j(A_F^{[N]})\delta_0, (A_F^{[N]} - z)^{-1} \delta_0 \rangle \delta_j.$$

As in the proof of Theorem 4.3, we conclude that (with $G_N(z) = \langle \delta_0, (A_F^{[N]} - z)^{-1} \delta_0 \rangle$),

$$\sum_{j=0}^{N-1} |Q_j(z) + G_N(z) P_j(z)|^2 = \frac{\mathrm{Im}\, G_N(z)}{\mathrm{Im}\, z} \, .$$

Thus, since $Q, P \in \ell_2$ if $G_N(z) \to G(z)$ through a subsequence, the limit $\zeta = G(z)$ obeys equality in (4.5). By Theorem 4.14, any such solution of the moment problem is a von Neumann solution. $\square$

We want to show that in many cases, $\lim f^{[N-1,N]}(z)$ will not exist. Consider a set of Stieltjes moments, $\{\gamma_n\}_{n=0}^\infty$ and the associated even Hamburger problem with moments

$$\Gamma_{2n} = \gamma_n, \qquad \Gamma_{2n+1} = 0. \tag{5.86}$$

Given $\rho \in \mathcal{M}^S(\gamma)$, let $\tilde\rho \in \mathcal{M}^H(\Gamma)$ be given by

$$d\tilde\rho(x) = \tfrac{1}{2}(\chi_{[0,\infty)}(x)\, d\rho(x^2) + \chi_{(-\infty,0]}(x)\, d\rho(x^2)) \tag{5.87}$$

so that Theorem 2.12 says that this sets up a one-one correspondence between even integrals in $\mathcal{M}^H(\Gamma)$ and $\mathcal{M}^S(\gamma)$. Let $\tilde{P}_n, \tilde{Q}_n$ be the orthogonal polynomials for Γ and P_n, Q_n, M_n, N_n for γ. Define d_n by $d_n^2 \int M_n(x)^2 x^{-1}\, d\rho(x) = 1$. Then we claim that

$$G_{\tilde{\rho}}(z) = zG_\rho(z^2) \tag{5.88}$$

$$\tilde{P}_{2n}(x) = P_n(x^2) \tag{5.89}$$

$$\tilde{P}_{2n-1}(x) = \frac{d_n M_n(x^2)}{x} \tag{5.90}$$

$$\tilde{Q}_{2n}(x) = xQ_n(x^2) \tag{5.91}$$

$$\tilde{Q}_{2n-1}(x) = d_n N_n(x^2). \tag{5.92}$$

To prove (5.89) and (5.90), we note that the right sides have the correct degree, and since $P_n(x^2)$ is even and $\frac{M_n(x^2)}{x}$ is odd, they are $d\tilde{\rho}$ orthogonal to each other. Easy calculations prove the $d\tilde{\rho}$ orthogonality of two $P_n(x^2)$'s and two $\frac{M_n(x^2)}{x}$'s. The formulae for $\tilde{Q}$ and $G_{\tilde{\rho}}$ follow by direct calculations using Theorem 4.2 for Q.

Theorem 5.30. *Let γ, Γ be related by* (5.86) *and let $d\tilde{\rho}^{(F)}, d\tilde{\rho}^{(K)}$ be the images of $d\rho_F, d\rho_K$ (for γ) under the map $\rho \mapsto \tilde{\rho}$ given by* (5.87). *Let $\tilde{f}^{[N,M]}(z)$ be the Padé approximants for $\sum_{n=0}^\infty (-1)^n \Gamma_n z^n$. Then*

$$\lim_{N\to\infty} \tilde{f}^{[2N-1,2N]}(z) = \int \frac{d\tilde{\rho}^{(F)}(x)}{1+xz} \tag{5.93}$$

$$\lim_{N\to\infty} \tilde{f}^{[2N,2N+1]}(z) = \int \frac{d\tilde{\rho}^{(K)}(x)}{1+xz}\,. \tag{5.94}$$

In particular, if the Γ problem is indeterminate, $\lim f^{[N-1,N]}(z)$ does not exist.

Proof. This follows directly from Theorem 6 for the γ problem and (5.88)–(5.92). $\square$

Of course, in the special case, the non-convergence of $f^{[N-1,N]}(z)$ is replaced by something almost as nice since the even and odd subsequences separately converge. But there is no reason to expect this to persist if Γ is not even and indeed, simple numerical examples ([14]) illustrate non-convergence is the rule. One can understand why this happens. In the indeterminate case, there is a one-parameter family of extensions, each with discrete spectrum. There is, in general, nothing to tack down $A_F^{[N]}$ so it wanders. In the even case, two self-adjoint extensions are even, one with an eigenvalue at 0 and one without, and the $A_F^{[N]}$ for odd N and even N track these. This suggests that $A_K^{[N]}$, which is tacked down to have a zero eigenvalue, should converge in strong resolvent sense and the corresponding $f^{[N,N]}$'s should converge. This is true and is not a previously known result:

Theorem 5.31. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Hamburger moments and let $\sum_{n=0}^\infty (-1)^n \gamma_n z^n$ be the associated series of Hamburger. Then the $f^{[N,N]}(z)$ Padé approximants exist if and only if*

$$P_N(0) \neq 0. \tag{5.95}$$

Moreover, (5.95) *holds if and only if there exists α_N so that the matrix $A_K^{[N+1]}$ given by* (5.2b) *has a zero eigenvalue, and then*

$$f^{[N,N]}(z) = (\delta_0, (1 + zA_K^{[N+1]})^{-1}\delta_0). \tag{5.96}$$

If $N \to \infty$ through the sequence of all N's for which (5.95) *holds, then*

$$\lim_{\substack{N\to\infty \\ N: P_N(0)\neq 0}} f^{[N,N]}(z) = \int \frac{d\rho(x)}{1+xz}\,, \tag{5.97}$$

where $d\rho$ is the unique solution of the moment problem in case it is determinate and the unique von Neumann solution with $\mu(\{0\}) > 0$ if the moment problem is indeterminate.

Remarks. 1. If $P_N(0) = 0$, then, by the second-order equation $P_N(0)$ obeys, we have that $P_{N+1}(0) \neq 0 \neq P_{N-1}(0)$, so (5.95) can fail at most half the time. Typically, of course, it always holds (e.g., under a small generic perturbation of the Jacobi matrix, one can prove that it will hold even if initially it failed).

2. If the γ's are a set of even moments, then (5.95) holds exactly for N even and

$$f^{[2M,2M]}(z) = \frac{z^{2M} Q_{2M+1}(-\frac{1}{z})}{z^{2M+1} P_{2M+1}(-\frac{1}{z})}\,,$$

so we get convergence of those measures we called $d\tilde\rho$ above.

3. The non-existence of $f^{[N,N]}$ is using the Baker definition that we have made. There is a classical definition which would define $f^{[N,N]}(z)$ even if $P_N(0) = 0$, (but (5.26) and (5.27) would both fail!). Under this definition, $f^{[N,N]}(z)$ would be $f^{[N-1,N-1]}(z)$ when $P_N(0) = 0$ and (5.97) would hold using all N rather than just those N with $P_N(0) \neq 0$.

Proof. Define

$$\widetilde{M}_N(z) = P_{N-1}(0)P_N(z) - P_N(0)P_{N-1}(z) \tag{5.98}$$

$$\tilde{N}_N(z) = P_{N-1}(0)Q_N(z) - P_N(0)P_{N-1}(z). \tag{5.99}$$

Then by the Wronskian calculations (see Proposition 4.1); also see (5.70)),

$$\tilde{N}_N(0) = \frac{1}{a_{N-1}} \neq 0 \tag{5.100}$$

$$\widetilde{M}_N'(0) = \sum_{j=0}^{N-1} \frac{P_j(0)^2}{a_{N-1}} \neq 0 \tag{5.101}$$

and, of course,

$$\widetilde{M}_N(0) = 0. \tag{5.102}$$

Define

$$A_N(z) = z^N \tilde{N}_{N+1}\left(-\tfrac{1}{z}\right) \tag{5.103}$$

$$B_N(z) = z^{N+1} \widetilde{M}_{N+1}\left(-\tfrac{1}{z}\right). \tag{5.104}$$

By (5.100), $\deg A_N = N$ and by (5.101/5.102), $\deg B_N = N$. Moreover, by the definition (5.98),

$$B_N(0) = 0 \Longleftrightarrow P_N(0) = 0 \tag{5.105}$$

and

$$B_N(0) = 0 \Longrightarrow P_N'(0) \neq 0 \tag{5.106}$$

since $P_N(0) = 0 \Rightarrow P_{N-1}(0) \neq 0$.

Moreover, we claim that

$$A_N(z) - B_N(z) \sum_{j=0}^{2N} \gamma_j z^j = O(z^{2N+1}). \tag{5.107}$$

This can be seen either by algebraic manipulation as in the remark following the proof of Theorem A.5 or by noting that we have proven it in (5.39) for Stieltjes measures. So if $\rho \in \mathcal{M}^H(\gamma)$ and μ_0 is a Stieltjes measure and $\rho_t = (1-t)\mu_0 + t\rho$, then $B_N(-z), A_N(-z)$ are real analytic functions of t and (5.107) is true for all small t in $(0,1)$ since $A_F^{[N+1]}(t) > 0$ for small t (and fixed N) and that is all the proof of (5.106) depends on.

If $P_N(0) \neq 0$, $B_N(0) \neq 0$, so $B^{[N,N]}(z) = \frac{B_N(z)}{B_N(0)}$ and $A^{[N,N]}(z) = \frac{A_N(z)}{B_N(0)}$ yield denominator and numerator of $f^{[N,N]}(t)$; so $f^{[N,N]}$ exists.

Moreover, the proof of Lemma 5.1 shows that an α_N exists giving $A_K^{[N+1]}$ a zero eigenvalue if and only if $P_N(0) \neq 0$. In that case, the proof of Proposition 5.8 is valid, and we have that (5.17) holds. Noting that $\frac{N_N}{M_N} = \frac{\tilde{N}_N}{\widetilde{M}_N}$, we see that (5.96) is then valid.

On the other hand, suppose that $P_N(0) = 0$ and that $f^{[N,N]}(z)$ exists. Then by (5.107), we have that

$$A_N(z) B^{[N,N]} - B_N(z) A^{[N,N]}(z) = O(z^{2N+1})$$

and so it is zero since the left side of this is of degree $2N$.

Since $P_N(0) = 0$, $\widetilde{M}_{N+1}(z) = -P_{N+1}(0) P_N(z) = c\widetilde{M}_N(z)$ where $c = -P_{N+1}(0)$ $P_{N-1}(0)^{-1}$, and similarly, $\tilde{N}_{N=1}(z) = c\tilde{N}_N(z)$. It follows that

$$A_N(z) = czA_{N-1}(z), \qquad B_N(z) = czB_{N-1}(z).$$

Thus, if $P_N(0) = 0$ but $f^{[N,N]}(z)$ exists, then

$$f^{[N,N]}(z) = f^{[N-1,N-1]}(z),$$

that is, the $[N-1, N-1]$ Padé approximant would need to have an error of order $O(z^{2N+1})$.

Since $P_N(0) = 0$, $A_K^{[N]} = A_F^{[N]}$ and so we would have that $\langle \delta_0, (A_F^{[N]})^j \delta_0 \rangle = \gamma_j$ for $j = 0, 1, \dots, 2N$. But as noted in the remark following the proof of Proposition 5.11, this can never happen. We conclude that if $P_N(0) = 0$, $f^{[N,N]}$ must fail to exist.

To complete the proof, define A_K to be $\bar{A}$ if the problem is determinate and the unique von Neumann extension with eigenvalue zero if the problem is indeterminate (so $A_K \pi(0) = 0$). Then the proof of Proposition 5.3 goes through without change and shows that $A_K^{[N]}$ converges to A_K in strong resolvent sense. This implies (5.97). $\square$

As for other $f^{[N+\ell-1,N]}(z)$ for series of Hamburger, we can only define $\gamma^{(j)}$ moment problems for j an even integer (positive or negative). This means that we can use (5.49)/(5.59) if ℓ is an even integer and (5.50)/(5.60) if ℓ is an odd integer. The result is the following:

Theorem 5.32. *Let $\{\gamma_n\}_{n=0}^\infty$ be a set of Hamburger moments and let $\sum_{n=0}^\infty (-1)^n \gamma_n z^n$ be the associated series of Hamburger. Then:*

(i) *If ℓ is any odd integer, the Padé approximants $f^{[N+\ell-1,N]}(z)$ exist if and only if $P_M^{(j)}(0) \neq 0$ where for $\ell > 0$, $j = \ell - 1$, and $M = N$ and if $\ell < 0$, $j = \ell + 1$ and $M = N + \ell - 1$. The functions that exist converge to a finite limit $f_\ell(z)$.*

(ii) *If ℓ is any even integer, the Padé approximants $f^{[N+\ell-1,N]}(z)$ all exist and lie in a compact subset in the topology of uniform convergence on compact subsets of $\mathbb{C}_+$. Any limit point, $f_\ell(z)$, is associated to a von Neumann solution, $\rho^{(\ell)}$, of the $\gamma^{(\ell)}$ moment problem via*

$$f_\ell(z) = \sum_{j=0}^{\ell-1} (-1)^j \gamma_j z^j + (-1)^\ell \gamma_\ell z^\ell \int_{-\infty}^\infty \frac{d\rho^{(\ell)}(x)}{1 + xz}$$

if $\ell > 0$ and

$$f_\ell(z) = \left\{ 1 - \gamma_1 z - \sum_{j=0}^{-\ell-1} (-1)^j \gamma_j^{(0)} z^{j+2} + (-1)^{\ell+1} \gamma_{-\ell}^{(0)} z^{-\ell+2} \int_{-\infty}^\infty \frac{d\rho^{(\ell)}(x)}{1 + xz} \right\}^{-1}$$

if $\ell < 0$. In particular, if the $\gamma^{(\ell)}$ problem is determinate, $f^{[N+\ell-1,N]}(z)$ is convergent.

(iii) *Let ℓ be an even integer. If the $\gamma^{(\ell)}$ problem is determinate (as a Hamburger problem), then for $\ell \geq 0$, $f_{\ell+1}(z) = f_\ell(z) = \cdots = f_0(z) = f_{-1}(z)$, and for $\ell \leq 0$, $f_{\ell-1}(z) = f_\ell(z) = \cdots = f_0(z) = f_1(z)$. In particular, if $|\gamma_j| \leq C^{j+1} j!$, then all $f^{[N+\ell-1,N]}(z)$ converges to the same ℓ-independent limits as $N \to \infty$.*

§6. Solutions of Finite Order

In this section, we will continue the analysis of the indeterminate Hamburger moment problem. Throughout, $\{\gamma_n\}_{n=0}^\infty$ will be a set of indeterminate Hamburger moments and ρ will be a solution of (1.1), the moment problem for γ.

We have picked out the von Neumann solutions as coming from self-adjoint extensions of the Jacobi matrix, A. But in a certain sense, every ρ does come from a self-adjoint extension of A! For let $\mathcal{H}_\rho = L^2(\mathbb{R}, d\rho)$, let $D(B) = \{f \in \mathcal{H}_\rho \mid \int x^2 |f(x)|^2 \, d\rho(x) < \infty\}$, and let

$$(Bf)(x) = xf(x).$$

Let $\mathbb{C}[X]$ be the set of polynomials in x which lies in $\mathcal{H}_\rho$ since all moments are finite, and let $\mathcal{H}_0 = \overline{\mathbb{C}[X]}$. Corollary 4.15 says that $\mathcal{H}_0 = \mathcal{H}_\rho$ if and only if ρ is a von Neumann solution. Let $A_\rho = B \restriction \mathbb{C}[X]$. Then to say ρ is a solution of the Hamburger moment problem is precisely to say that A_ρ is unitarily equivalent to the Jacobi matrix, A, associated to γ under the natural map (so we will drop the subscript ρ). In that sense, B is a self-adjoint extension of A, but not in the von Neumann sense.

B is minimal in the sense that there is no subspace of $\mathcal{H}_\rho$ containing $\mathcal{H}_0$ and left invariant by all bounded functions of B (equivalently, left invariant by all $(B - z)^{-1}$, $z \in \mathbb{C} \backslash \mathbb{R}$ or by all e^{iBs}, $s \in \mathbb{R}$). So (if ρ is not a von Neumann extension) we are in the strange situation where $D(B) \cap \mathcal{H}_0$ is dense in $\mathcal{H}_0$, $B[D(B) \cap \mathcal{H}_0] \subset \mathcal{H}_0$, but $\mathcal{H}_0$ is not invariant for the resolvents of B!

It is not hard to see that the set of all solutions of the moment problem is precisely the set of all self-adjoint "extensions" of A in this extended sense, which are minimal ($\mathcal{H}_0$ is cyclic for B) and modulo a natural unitary equivalence. This is a point of view originally exposed by Naimark [24, 25, 26, 27] and developed by Livsic [21], Gil de Lamadrid [7], and Langer [20]. See the discussion of Naimark's theory in Appendix 1 of [2].

In the language of Cayley transforms, the extensions associated to ρ's that we will call of order at most n below are parametrized by unitary maps, U, from $\mathcal{K}_+ \oplus \mathbb{C}^n$ to $\mathcal{K}_- \oplus \mathbb{C}^n$ with U_1, U_2 equivalent if and only if there is a unitary map $V : \mathbb{C}^n \to \mathbb{C}^n$ so $U_1(1 \oplus V) = (1 \oplus V)U_2$. From this point of view, these extensions are then parametrized by the variety of conjugacy classes of $\mathcal{U}(n+1)$ modulo a $\mathcal{U}(n)$ subgroup. This has dimension $(n+1)^2 - n^2 = 2n+1$. Our parametrization below in terms of a ratio of two real polynomials of degree at most n also is a variety of dimension $2n+1$, showing the consistency of the parametrization. (The ρ's of exact order n will be a manifold.)

Given any ρ, we define the *order* of ρ,

$$\operatorname{ord}(\rho) = \dim(\mathcal{H}_\rho / \mathcal{H}_0)$$

so the von Neumann solutions are exactly the solutions of order 0. Our main result in this section will describe all solutions of finite order which turn out to correspond precisely to those ρ's whose Nevanlinna function Φ_ρ are ratios of real polynomials.

They will also be ρ's for which $d\rho / \prod_{i=1}^n |x - z_i|^2$ is the measure of a determinate moment problem. We will therefore need some preliminaries about such problems. Given

$z_1, \dots, z_n \in \mathbb{C}_+$, by using partial fractions we can write for x real,

$$\frac{x^m}{\prod_{i=1}^n |x-z_i|^2} = P_{m-2n}(x; z_1, \dots, z_n) + \sum_{i=1}^n \biggl[\frac{z_i^m}{z_i - \bar z_i} \, \frac{1}{x-z_i} + \frac{\bar z_i^m}{\bar z_i - z_i} \, \frac{1}{x-\bar z_i} \biggr] \tag{6.1}$$

where P_{m-2n} is a polynomial in x of degree $m-2n$. To see (6.1), write $\prod_{i=1}^n |x-z_i|^2 = \prod_{i=1}^n (x-z_i)(x-\bar z_i)$ and analytically continue. The sum in (6.1) comes from computing the residues of the poles of these functions. Define

$$\Gamma_m^{(0)}(z_1, \dots, z_n) = E_x^\gamma(P_{m-2n}(x; z_1, \dots, z_n)), \tag{6.2}$$

where, as usual, E_x^γ is the expectation with respect to any solution of the moment problem. For $\zeta_1, \dots, \zeta_n \in \mathbb{C}_+$, let

$$\Gamma_m(z_1, \dots, z_n; \zeta_1, \dots, \zeta_n) = \Gamma_m^{(0)}(z_1, \dots, z_n) + \sum_{i=1}^n \biggl[\frac{z_i^m}{z_i - \bar z_i} \, \zeta_i + \frac{\bar z_i^m}{\bar z_i - z_i} \, \bar\zeta_i \biggr]. \tag{6.3}$$

Theorem 6.1. *Fix $z_1, \dots, z_n$ and $\zeta_i, \dots, \zeta_n$ in $\mathbb{C}_+$. There is a one-one correspondence between $\nu \in \mathcal{M}^H(\Gamma(z_1, \dots, z_n; \zeta_1, \dots, \zeta_n))$ and those ρ in $\mathcal{M}^H(\gamma)$ which obey*

$$\int \frac{d\rho(x)}{x-z_i} = \zeta_i, \qquad i = 1, \dots, n \tag{6.4}$$

under the association

$$d\rho(x) \leftrightarrow d\nu(x) = \prod_{i=1}^n |x-z_i|^{-2} \, d\rho(x). \tag{6.5}$$

That is, ρ has moments $\{\gamma_m\}_{m=0}^\infty$ with subsidiary conditions (6.4) *if and only if ν given by* (6.5) *has the moments $\{\Gamma_m(z_1, \dots, z_n; \zeta_1, \dots, \zeta_n)\}_{m=0}^\infty$.*

Proof. This is pure algebra. The functions $\{x_m\}_{m=0}^\infty$, $\{\frac{1}{x-z_i}\}_{i=1}^n$ are linearly independent as analytic functions (finite sums only). (6.1) says that each function $x^m / \prod_{i=1}^n (x - z_i)(x-\bar z_i) \equiv Q_m(x)$ is in the span, $\mathcal{S}$, of these functions. On the other hand, since $\prod_{i=1}^n (x-z_i)(x-\bar z_i) \equiv L(x)$ is a polynomial in x, and $x^\ell Q_m(x) = Q_{\ell+m}(x)$, $L(x)Q_m(x)$ is in the span of the $\{Q_m(x)\}$. Similarly, since $\frac{L(x)}{(x-z_i)}$ is a polynomial, $L(x)Q_0(x)\frac{1}{(x-z_i)}$ lies in that span.

Thus, $\{Q_m(x)\}$ is also a basis of $\mathcal{S}$. It follows that there is a one-one correspondence between assignments of numbers $Q_m(x) \mapsto \Gamma_m$ and of assignments $x^m \mapsto \gamma_m$, $\frac{1}{x-z_i} \mapsto \zeta_i$, $\frac{1}{x-\bar z_i} \mapsto \lambda_i$ since each defines a linear functional on $\mathcal{S}$. For the linear functional to be real in Γ_m representation, all Γ_m must be real. For reality in (γ, ζ, λ) representation, we must have γ_m real and $\lambda_i = \bar\zeta_i$. (6.3) is just an explicit realization of the map from $\gamma, \zeta, \bar\zeta$ to Γ. Thus, a real $d\rho$ has moments γ_m with ζ_i conditions if and only if $\int x^m \prod_{i=1}^n |x-z_i|^{-2} \, d\rho(x) = \Gamma_m$ for all m. Since (6.5) shows ν is positive if and only if ρ is, we see that the claimed equivalence holds. $\square$

As an aside of the main theme of this section, we can construct determinate Hamburger moments quite close to indeterminate ones. The result is related to Corollary 4.21.

Theorem 6.2. *Let $\{\gamma_n\}_{n=0}^{\infty}$ be a set of Hamburger moments. Then for any $a \in (0,\infty)$, there is a c_a so that the moment problem with moments*

$$\begin{aligned}\tilde\gamma_{2n+1} &= 0\\ \tilde\gamma_{2n} &= \gamma_{2n} - a^2\gamma_{2n-2} + a^4\gamma_{2n-2} + \cdots + (-1)^n a^{2n}\gamma_0 + (-1)^{n+1}c_a a^{2n+2}\end{aligned} \tag{6.6}$$

is a determinate moment problem.

Proof. Let ρ_1 be any solution for the Hamburger problem. Since $\frac{1}{2}[d\rho_1(x)+d\rho_1(-x)] = d\tilde\rho$ has moments

$$\int x^m\, d\tilde\rho(x) = \begin{cases} 0 & m \text{ odd} \\ \gamma_{2m} & m \text{ even}\end{cases} \equiv \gamma'_{2m},$$

we can suppose $\gamma_{2m+1} = 0$. Let ρ be a von Neumann solution to the γ'_m moment problem which is invariant under $x \to -x$. If the γ'_m problem is determinate, then the unique solution is invariant. Otherwise, this follows from the proof of Theorem 2.13. Let $d\mu(x) = \frac{d\rho(x)}{1+a^2x^2}$. By Corollary 4.15 and Theorem 6.1, ρ is the unique solution of the γ' moment problem with $\int \frac{d\rho(x)}{x-ia^{-1}} \equiv \zeta_{a^{-1}}$. Thus, the $\Gamma_m(ia^{-1},\zeta_{a^{-1}})$ problem is determinate. If $c_a = a^{-1}\operatorname{Im}\zeta_{a^{-1}}$, then a calculation using the geometric series with remainder shows that $\Gamma_m(-ia^{-1},\zeta_{a^{-1}}) = \tilde\gamma_m$ given by (6.6). $\square$

Returning to the main theme of this section, we next examine when a Herglotz function is a real rational function. Define for $z \in \mathbb{C}_+$,

$$\varphi_z(x) \equiv \frac{1+xz}{x-z} \tag{6.7a}$$

viewed as a continuous function on $\mathbb{R}\cup\{\infty\}$ with

$$\varphi_z(\infty) = z. \tag{6.7b}$$

If $d\sigma(x) = [\frac{d\mu(x)}{1+x^2}] + c\delta_\infty$ as a finite measure on $\mathbb{R}\cup\{\infty\}$, then (1.19) can be rewritten as

$$\Phi(z) = d + \int_{\mathbb{R}\cup\{\infty\}} \varphi_z(x)\, d\sigma(x). \tag{6.8}$$

If $\sigma(\{\infty\}) = 0$ and $\int |x|\, d\sigma(x) < \infty$, define $\tilde d = d - \int x\, d\sigma(x)$.

Proposition 6.3. *A Herglotz function is a ratio of two real polynomials if and only if the representation (6.8) has a σ with finite support. If σ has exactly N points in its support, there are three possibilities for the degrees of P, Q in $\Phi(z) = \frac{P(z)}{Q(z)}$ with P, Q relatively prime polynomials:*

(i) $(\sigma(\{\infty\}) = 0, \tilde d = 0)$, $\deg P = N-1$, $\deg Q = N$
(ii) $(\sigma(\{\infty\}) = 0, \tilde d \neq 0)$, $\deg P = \deg Q = N$
(iii) $(\sigma(\{\infty\}) \neq 0)$, $\deg P = N$, $\deg Q = N-1$

In all cases, we say $N = \max(\deg(P), \deg(Q))$ *is the degree of* Φ.

Proof. Elementary. $\square$

Remark. The set of σ's with exactly N pure points is a manifold of dimension $2N$ (N points, N weights). $d \in \mathbb{R}$ is another parameter so the set of such Φ's is a manifold of dimension $2N+1$.

As a final preliminary, for any $z \in \mathbb{C}\backslash\sigma(B) \equiv \mathbb{C}\backslash \operatorname{supp}(d\rho)$ and $n = 1, 2, \dots,$ we introduce the functions $e_n(z)$ on $\operatorname{supp}(d\rho)$,

$$e_n(z)(x) = \frac{1}{(x-z)^n},$$

thought of as elements of $\mathcal{H}_\rho = L^2(\mathbb{R}, d\rho)$.

The main result of this section is:

Theorem 6.4. *Let* γ *be a set of indeterminate Hamburger moments and let* $\rho_0 \in \mathcal{M}^H(\gamma)$. *Fix* $N \in \{0, 1, \dots\}$. *Then the following are equivalent:*

(1) ρ_0 *has order at most* N.
(2) *For some set of distinct* $z_1, \dots, z_N \in \mathbb{C}\backslash\mathbb{R}$, $\mathcal{H}_0 \cup \{e_1(z_j)\}_{j=1}^N$ *span* $\mathcal{H}_{\rho_0}$.
(3) *For any set of distinct* $z_1, \dots, z_N \in \mathbb{C}\backslash\mathbb{R}$, $\mathcal{H}_0 \cup \{e_1(z_j)\}_{j=1}^N$ *span* $\mathcal{H}_{\rho_0}$.
(4) *For some* $z_0 \in \mathbb{C}\backslash\mathbb{R}$, $\mathcal{H}_0 \cup \{e_j(z_0)\}_{j=1}^N$ *span* $\mathcal{H}_{\rho_0}$.
(5) *For any* $z_0 \in \mathbb{C}\backslash\mathbb{R}$, $\mathcal{H}_0 \cup \{e_j(z_0)\}_{j=1}^N$ *span* $\mathcal{H}_{\rho_0}$.
(6) *For some set of* $z_0, z_1, \dots, z_N \in \mathbb{C}_+$ *and* $\zeta_j = G_{\rho_0}(z_j)$, *there is no other* $\rho \in \mathcal{M}^H(\gamma)$ *with* $G_\rho(z_j) = \zeta_j$.
(7) *For all sets of* $z_0, z_1, \dots, z_N \in \mathbb{C}_+$ *and* $\zeta_j = G_{\rho_0}(z_j)$, *there is no other* $\rho \in \mathcal{M}^H(\gamma)$ *with* $G_\rho(z_j) = \zeta_j$.
(8) *For some* $z_0, z_1, \dots, z_N \in \mathbb{C}_+$ *and* $\zeta_j = G_{\rho_0}(z_j)$, *the* $\Gamma(z_0, \dots, z_N; \zeta_0, \dots, \zeta_N)$ *moment problem is determinate.*
(9) *For any* $z_0, z_1, \dots, z_N \in \mathbb{C}_+$ *and* $\zeta_j = G_{\rho_0}(z_j)$, *the* $\Gamma(z_0, \dots, z_N; \zeta_0, \dots, \zeta_N)$ *moment problem is determinate.*
(10) *For some* $z_1, \dots, z_N \in \mathbb{C}_+$ *and* $\zeta_j = G_{\rho_0}(z_j)$, ρ_0 *is a von Neumann solution of the* $\Gamma(z_1, \dots, z_N; \zeta_1, \dots, \zeta_N)$ *moment problem.*
(11) *For any* $z_1, \dots, z_N \in \mathbb{C}_+$ *and* $\zeta_j = G_{\rho_0}(z_j)$, ρ_0 *is a von Neumann solution of the* $\Gamma(z_1, \dots, z_N; \zeta_1, \dots, \zeta_N)$ *moment problem.*
(12) *The Nevanlinna function* Φ *of* ρ_0 *is a rational function of degree at most* N.

In particular, the Nevanlinna function Φ *of* ρ_0 *has degree* N *if and only if* ρ_0 *has order* N. *Moreover, if one and hence all those conditions hold,* ρ_0 *is an extreme point in* $\mathcal{M}^H(\gamma)$ *and is also a pure point measure.*

Remark. The measures obeying (1)–(12) are what Akhiezer calls canonical solutions of order N.

Lemma 6.5. *If* $\varphi \in \mathcal{H}_0$ *and* $z \notin \sigma(B)$, *then*

$$(B-z)^{-1}\varphi \in \mathcal{H}_0 + [e_1(z)].$$

Proof. Since $(B-z)^{-1}$ is bounded and $\mathcal{H}_0 + [e_1(t)]$ is closed, it suffices to prove this for $\varphi(x) = P(x)$, a polynomial in x. But then

$$\begin{aligned}(B-z)^{-1}\varphi = (x-z)^{-1}P(x) &= P(z)(x-z)^{-1} + \frac{(P(x)-P(z))}{x-z} \\ &= P(z)e_1(z) + R(x)\end{aligned}$$

for a polynomial R, that is, $(B-z)^{-1}\varphi \in \mathcal{H}_0 + e_1(z)$. $\square$

Lemma 6.6. *Supose that $z_0, z_1, \dots, z_\ell \in \mathbb{C}\backslash\sigma(B)$ are distinct. If $e_m(z_0)$ is in the span of $\mathcal{H}_0 \cup \operatorname{span}[\{e_j(z_0)\}_{j=1}^{m-1}] \cup \operatorname{span}[\{e_1(z_k)\}_{k=1}^{\ell}]$, then so is $e_{m+1}(z_0)$.*

Remark. ℓ can be zero.

Proof. By hypothesis, for some $\varphi \in \mathcal{H}_0$ and $\{\alpha_j\}_{j=1}^{m-1}$ and $\{\beta_k\}_{k=1}^{\ell}$ in $\mathbb{C}$,

$$e_m(z_0) = \varphi + \sum_{j=1}^{m-1} \alpha_j e_j(z_0) + \sum_{k=1}^{\ell} \beta_k e_1(z_k).$$

Apply $(B-z_0)^{-1}$ to this using $(B-z_0)^{-1}e_j(z_0) = e_{j+1}(z_0)$, Lemma 6.5, and $(B-z_0)^{-1}e_1(z_k) = (z_0-z_k)^{-1}[e_1(z_0) - e_1(z_k)]$ and we see that $e_{m+1}(z_0)$ is in the requisite span. $\square$

Proposition 6.7. *Let $\ell = \operatorname{ord}(\rho) < \infty$. Then for any set $\{z_i\}_{i=1}^{\ell}$ of ℓ distinct points in $\mathbb{C}\backslash\sigma(B)$, $\mathcal{H}_0 \cup \{e_1(z_i)\}_{i=1}^{\ell}$ span $\mathcal{H}_\rho$.*

Proof. By the Stone-Weierstrass theorem, linear combinations of $\{(x-z)^{-1} \mid z \in \mathbb{C}\backslash\sigma(B)\}$ are dense in the continuous functions on $\sigma(B)$ vanishing at infinity, and so they are dense in $L^2(\mathbb{R}, d\rho)$. It follows that we can find $\{z_i\}_{i=1}^{\ell}$ so that $\mathcal{H}_0 \cup \{e_1(z_i)\}_{i=1}^{\ell}$ span $\mathcal{H}_\rho$.

Pick $z_0 \in \mathbb{C}\backslash\sigma(B)$ and let $W = (B-z_\ell)(B-z_0)^{-1}$. Then W is bounded with bounded inverse, so it maps dense subspaces into dense subspaces. By Lemma 6.5, $W[\mathcal{H}_0] \subset \mathcal{H}_0 + [e_1(z_0)]$. For $i = 1, \dots, \ell-1$, $We_1(z_i) = e_1(z_i) + (\frac{z_0-z_\ell}{z_0-z_i})[e_1(z_0) - e_1(z_i)]$ and $We_1(z_\ell) = e_1(z_0)$. Thus, W maps the span of $\{e_1(z_i)\}_{i=1}^{\ell}$ into $\{e_1(z_i)\}_{i=0}^{\ell-1}$. So $\mathcal{H}_0 \cup \{e_1(z_i)\}_{i=0}^{\ell-1}$ span $\mathcal{H}_\rho$. By successive replacement, we can move the z_i's to an arbitrary set of distinct points. $\square$

Remark. Proposition 6.7 shows (1)–(3) of Theorem 6.4 are equivalent.

Proposition 6.8. *Suppose that $\ell = \operatorname{ord}(\rho) < \infty$. Then for any $z_0 \in \mathbb{C}\backslash\sigma(B)$, $\mathcal{H}_0 \cup \{e_j(z_0)\}_{j=1}^{\ell}$ span $\mathcal{H}_\rho$.*

Proof. By hypothesis, there must be some dependency relation

$$\varphi + \sum_{j=1}^{\ell+1} \alpha_j e_j(z_0) = 0 \tag{6.10}$$

for $\varphi \in \mathcal{H}_0$ and some $(\alpha_1, \dots, \alpha_{\ell+1}) \neq 0$. Let $k+1 = \max\{j \mid \alpha_j \neq 0\}$. Then solving (6.10) for $e_{k+1}(z_0)$, we see that $e_{k+1}(z_0)$ lies in the span of $\mathcal{H}_0 \cup \{e_j(z_0)\}_{j=1}^k$; and so by induction and Lemma 6.6, all $e_m(z_0)$ lie in this span and so in the span of $\mathcal{H}_0 \cup \{e_j(z_0)\}_{j=1}^\ell$. $e_1(z)$ is an analytic function in $\mathbb{C}\backslash\mathbb{R}$ with Taylor coefficients at z_0 equal to $e_n(z_0)$, so $e_1(z)$ lies in the span of $\mathcal{H}_0 \cup \{e_j(z_0)\}_{j=1}^\ell$ for z in the same half plane as z_0. By Proposition 6.7, these e_1's together with $\mathcal{H}_0$ span $\mathcal{H}_\rho$. $\square$

Remark. Proposition 6.8 shows that (1), (4), (5) of Theorem 6.4 are equivalent.

Proposition 6.9. *Fix distinct points $z_1, \dots, z_\ell \in \mathbb{C}\backslash\mathbb{R}$. Let*

$$d\mu(x) = \prod_{i=1}^{\ell} |x - z_i|^{-2} \, d\rho(x).$$

Then the polynomials are dense in $L^2(\mathbb{R}, d\mu)$ if and only if $\mathcal{H}_0 \cup \{e_1(z_j)\}_{j=1}^\ell$ span $\mathcal{H}_\rho$.

Proof. Let U be the unitary map from $\mathcal{H}_\rho$ to $\mathcal{H}_\mu$ given by

$$(Uf)(x) = \prod_{i=1}^{\ell} (x - z_i) f(x).$$

Then U maps the span of $\mathbb{C}[X] \cup \{e_1(z_i)\}_{i=1}^\ell$ onto $\mathbb{C}[X]$ for $P(x)$ is a polynomial of degree m if and only if $\prod_{i=1}^\ell (x-z)^{-1} P(x)$ is a linear combination of a polynomial of degree $\max(0, m-\ell)$ and $\{(x-z_i)^{-1}\}_{i=1}^\ell$. Thus, the density assertions are equivalent. $\square$

Remark. Proposition 6.9 and Corollary 4.15 show the equivalence of (2), (3), (10), and (11) of Theorem 6.4 (given that we already know that (2) and (3) are equivalent).

Proposition 6.10. *If* $\mathrm{ord}(\rho_0)$ *is finite, then ρ_0 is a pure point measure with discrete support.*

Proof. Let $\ell = \mathrm{ord}(\rho_0)$. Pick distinct $\{z_i\}_{i=1}^\ell$ in $\mathbb{C}_+$. Then by Propositions 6.7 and 6.9, the polynomials are dense in $L^2(\mathbb{R}, d\mu_\ell)$ where for $k = 0, 1, \dots, \ell$, we set

$$d\mu_k(x) = \prod_{j=1}^{k} |x - z_i|^{-2} \, d\rho(x).$$

Let k_0 be the smallest k for which the polynomials are dense in $L^2(\mathbb{R}, d\mu_k)$. If $k_0 = 0$, then $d\rho$ is a von Neumann solution of the γ problem. If $k_0 > 0$, then $d\mu_{k_0-1}$ is not a von Neumann solution of its moment problem. So by Proposition 4.15 and Theorem 6.1, the moment problem for $\Gamma_m^{(0)} \equiv \Gamma_m(z_1, \dots, z_{k_0-1}, z_{k_0}; \zeta_1, \dots, \zeta_{k_0-1}, \zeta_k)$ is indeterminate. But since the polynomials are dense in $L^2(\mathbb{R}, d\mu_k)$, $d\mu_{k_0}$ is a von Neumann solution of an indeterminate problem.

Either way, $d\mu_{k_0}$ is a von Neumann solution of an indeterminate problem. It follows Theorem 4.11 that $d\mu_{k_0}$ and so $d\rho$ is a discrete point measure. $\square$

As a final preliminary to the proof of Theorem 6.4, we need a known result about interpolation of Herglotz functions. Given $z_1, \dots, z_n; w_1, \dots, w_n \in C_+$ with the z's distinct, define the $n \times n$ matrix D by

$$D_{ij}(z_1, \dots, z_n; w_1, \dots, w_n) = \frac{w_i - \bar{w}_j}{z_i - \bar{z}_j}\,. \tag{6.11}$$

Theorem 6.11. *Pick $z_1, \dots, z_n \in \mathbb{C}_+$ with $n \geq 1$. There exists a Herglotz function Φ with*

$$\Phi(z_i) = w_i, \qquad i = 1, \dots, n \tag{6.12}$$

if and only if $D(z_1, \dots, z_n; w_1, \dots, w_n)$ is a (not necessarily strictly) positive definite matrix. Moreover, the following are equivalent, given such a Φ:

(1) $\det D(z_1, \dots, z_n; w_1, \dots, w_n) = 0$.
(2) *There is a unique Herglotz function Φ obeying* (6.12).
(3) *Φ is a real rational polynomial of degree at most $n-1$.*

Remark. Since (3) is independent of the choice of $\{z_i\}_{i=1}^n$, so are (1), (2).

We will sketch a proof of this result (fleshing out some arguments in [1]) below.

Proof of Theorem 6.4. As already noted, Propositions 6.7, 6.8, and 6.9 show that (1), (2), (3), (4), (5), (10), and (11) are equivalent. Theorem 6.1 and Corollary 4.15 prove the equivalence of (10) and (11) with (6), (7), (8), and (9). By Theorems 4.14 and 6.11, (6) and (12) are equivalent.

Since $\operatorname{ord}(\rho) = N$ is equivalent to $\operatorname{ord}(\rho) \geq N$ and the negation of $\operatorname{ord}(\rho) \leq N-1$, we see that Φ_{ρ_0} has degree precisely equal to $\operatorname{ord}(\rho_0)$. That ρ_0 is then an extreme point is proven in Appendix B. $\square$

We conclude this section by proving Theorem 6.11.

Proposition 6.12. *Let Φ be a Herglotz function and let $w_i = \Phi(z_i)$, $i = 1, \dots, n$ for distinct $z_1, \dots, z_n \in \mathbb{C}_+$. Let D be given by* (6.11). *Then $D(z_1, \dots, z_n; w_1, \dots, w_n)$ is (not necessarily strictly) positive definite and* $\det D = 0$ *if and only if Φ is a real ratio of polynomials of degree $n-1$ or less.*

Proof. Using the Herglotz representation (1.19), we get a representation of D_{ij},

$$\frac{w_i - \bar{w}_j}{z_i - \bar{z}_j} = c + \int d\mu(x)\, \frac{1}{x - z_i}\, \frac{1}{x - \bar{z}_j}\,,$$

from which we obtain for $\alpha \in \mathbb{C}^N$:

$$\sum_{i,j=1}^n \bar{\alpha}_i \alpha_j D_{ij} = c \left| \sum_{i=1}^n \alpha_j \right|^2 + \int_{-\infty}^{\infty} d\mu(x) \left| \sum_{i=1}^n \frac{\alpha_i}{x_i - z_i} \right|^2, \tag{6.13}$$

proving the positivity.

Suppose $\det(D) = 0$. Then there is a non-zero $\alpha \in \mathbb{C}^n$ so that the right side of (6.13) is 0. Note that $\sum_{i=1}^n \frac{\alpha_i}{(x-z_i)} = \prod_{i=1}^n (x-z_i)^{-1} Q(x)$, where Q is a polynomial of degree $n-1$ if $\sum_{i=1}^n \alpha_i \neq 0$ and of degree at most $n-2$ if $\sum_{i=1}^n \alpha_i = 0$. Thus, for the right side of (6.13) to vanish for some non-zero α in $\mathbb{C}^n$, either $c \neq 0$ and μ is supported at $n-2$ or fewer points, or else $c = 0$ and μ is supported at $n-1$ or fewer points. Either way, by Proposition 6.3, Φ is a real rational function of degree at most $n-1$.

Conversely, suppose Φ is a real rational function of degree precisely $n-1$. Then either μ is supported at $n-1$ points (say, $x_1, \dots, x_{n-1}$) or $c \neq 0$ and μ is supported at $n-2$ points (say, $x_1, \dots, x_{n-2}$). The map $\psi : \mathbb{C}^n \to \mathbb{C}^{n-1}$ given by

$$\psi_j(\alpha) = \sum_{i=1}^n \frac{\alpha_i}{x_j - z_i}$$

(with $\psi_{n-1}(\alpha) = \sum_{i=1}^n \alpha_i$ if $c \neq 0$) has a non-zero kernel by dimension counting. Thus, the right side of (6.13) is zero for some $\alpha \in \mathbb{C}^N$. If degree Φ is smaller than $n-1$, we can find $(\alpha_1, \dots, \alpha_\ell) \in \mathbb{C}^\ell$ so that $\sum_{i,j=1}^\ell \bar{\alpha}_i \alpha_j D_{ij} = 0$, which still implies that $\det(D) = 0$. $\square$

Proposition 6.13. *Let $z_1, \dots, z_n; w_1, \dots, w_n$ lie in $\mathbb{C}_+$ with the z_i distinct. Suppose the matrix D_{ij} given by* (6.11) *is* (*not necessarily strictly*) *positive definite. Then there exists a Herglotz function with $\Phi(z_i) = w_i$, $i = 1, \dots, n$.*

Proof. This is a fairly standard use of the Hahn-Banach theorem. We will use the representation (6.8) for Φ and the function φ_z of (6.7). Begin by noting that without loss of generality, we can suppose $z_n = i$ (by mapping $\mathbb{C}_+ \to \mathbb{C}_+$ with a linear map that takes the original z_n to i) and that $\operatorname{Re} w_n = 0$ (by adjusting the constant d in (6.8)). Indeed, since

$$\varphi_i(x) \equiv i, \tag{6.14}$$

this choice $\operatorname{Re}\Phi(i) = 0$ is equivalent to $d = 0$ in the representation (6.8).

Let V be the $2n-1$-dimensional subspace of $C(\mathbb{R} \cup \{\infty\})$, the real-valued continuous functions on $\mathbb{R} \cup \{\infty\}$ spanned by 1, $\{\operatorname{Re}\varphi_{z_j}(\,\cdot\,)\}_{j=1}^{n-1}$ and $\{\operatorname{Im}\varphi_{z_j}(\,\cdot\,)\}_{j=1}^{n-1}$. Any $f \in V$ can be written:

$$f = A_n + \sum_{j=1}^{n-1} A_j \varphi_j(x) + \bar{A}_j \, \overline{\varphi_j(x)} \tag{6.15}$$

with $A_1, \dots, A_{n-1} \in \mathbb{C}$ and $A_n \in \mathbb{R}$. Define a linear functional $f : V \to \mathbb{R}$ by

$$\ell(f) = A_n \operatorname{Im} w_n + \sum_{j=1}^{n-1} A_j w_j + \bar{A}_j \bar{w}_j \tag{6.16}$$

if f has the form (6.15).

We will prove shortly that

$$f(x) > 0 \qquad \text{for all } x \Rightarrow \ell(f) > 0. \tag{6.17}$$

Assuming this, we let $X = \{f \in C(\mathbb{R} \cup \{\infty\} \mid f(x) > 0 \text{ for all } x\}$ and $Y = \{f \in V \mid \ell(f) = 0\}$. Since X is open and Y closed, by the separating hyperplane version of the Hahn-Banach theorem (see [33]), there is a linear functional L on $\mathbb{C}(\mathbb{R} \cup \{\infty\})$ so $L > 0$ on X and $L \leq 0$ on Y. If L is normalized so $L(1) = \operatorname{Im} w_n$, it is easy to see that L extends ℓ, and so defines a measure σ on $\mathbb{R} \cup \{\infty\}$ with

$$\Phi(z_i) \equiv \int \varphi_{z_i}(x)\, d\sigma(x) = w_i, \qquad i = 1, \dots, n.$$

Thus, if (6.17) holds, we have the required Φ.

Since $f(x) > 0$ on the compact set $\mathbb{R} \cup \{\infty\}$ implies $f \equiv \varepsilon + g$ with $g \geq 0$ and $\varepsilon > 0$ (by hypothesis, $1 \in V$) and $\operatorname{Im} w_n > 0$, we need only show $f \geq 0$ implies $\ell(f) \geq 0$.

If f has the form (6.15), we can write

$$f(x) = \frac{Q(x)}{\prod_{j=1}^{n-1} |x - z_j|^2}\,,$$

where Q is a polynomial. $f \geq 0$ implies $Q \geq 0$. Any real non-negative polynomial has roots either in complex conjugate pairs or double real roots, so Q must have even degree and have the form

$$Q(x) = c^2 \prod_{k=1}^{\ell} |x - y_k|^2$$

for suitable $y_1, \dots, y_\ell \in \mathbb{R} \cup \mathbb{C}_+$. Thus, with $R(x) = c \prod_{k=1}^{\ell} (x - y_k)$,

$$f = |h|^2 \qquad \text{with} \qquad h(x) = \frac{R(x)}{\prod_{j=1}^{n-1} (x - z_j)}\,.$$

Since f is bounded on $\mathbb{R} \cup \{\infty\}$, $\deg(R) \leq n - 1$, and thus h has the form

$$h(x) = \beta_n + \sum_{j=1}^{n-1} \beta_j (x - z_j)^{-1}. \tag{6.18}$$

Since $(x - z_j)^{-1} = (z_j - i)^{-1}[\frac{(x-i)}{(x-z_j)} - 1]$, we can rewrite (6.18) as

$$h(x) = \sum_{j=1}^{n} \alpha_j \, \frac{x - i}{x - z_j}$$

for real x. Thus,

$$f(x) = |h(x)|^2 = \sum_{j=1}^{n} \bar{\alpha}_i \alpha_j \frac{x^2 + 1}{(x - \bar{z}_j)(x - z_j)} = \sum_{j=1}^{n} \bar{\alpha}_i \alpha_j \left[\frac{\varphi_{z_j}(x) - \overline{\varphi_{z_i}(x)}}{z_j - \bar{z}_i} \right]$$

so that

$$\ell(f) = \sum_{i,j=1}^{n} \bar{\alpha}_i \alpha_j D_{ij},$$

which is non-negative by hypothesis. $\square$

Proof of Theorem 6.11. The first assertion is a direct consequence of Propositions 6.12 and 6.13. Proposition 6.12 shows the equivalence of (1) and (3).

To prove (1) $\Rightarrow$ (2), suppose (1) holds and, as in the last proof, we can suppose that $z_n = i$ and $\operatorname{Re} w_n = 0$. Then by our proof of Proposition 6.12, the set of points where the measure σ of (6.8) is supported is determined by the α with $\sum_i D_{ij}\alpha_j = 0$ as an $n-1$ point set $x_1, \dots, x_{n-1}$ (with $x_{n-1} = \infty$ allowed). Thus, any such Φ is of the form P/Q where $\deg(P) \leq n-1$ and $Q(z) = \prod_{j=1}^{n-1}(z - x_j)$ (if $x_{n-1} = \infty$, the product only goes from 1 to $n-2$), If Φ_1 and Φ_2 are two solutions of (6.12), they have the same Q but they could be distinct P's, say P_1 and P_2. But by (6.12), $P_1(z) - P_2(z)$ vanishes at $z_1, \dots, z_n$. Since $P_1 - P_2$ is a polynomial of degree $n-1$, this is only possible if $P_1 - P_2 = 0$, that is, $\Phi_1 = \Phi_2$. Thus, (1) $\Rightarrow$ (2).

For the converse, suppose the determinant

$$D(z_1, \dots, z_n; w_1, \dots, w_n) > 0. \tag{6.19}$$

If $n = 1$, since $z, w \in \mathbb{C}_+$, it is easy to see there are multiple Φ's obeying (6.12). (For example, as usual we can consider the case $z = w = i$ and then that $\Phi(z) = z$ or $\Phi(z) = -z^{-1}$.) So we suppose $n \geq 2$.

Consider the function $g(w) = \det[D(z_1, \dots, z_n; w_1, \dots, w_{n-1}, w)]$ where we vary w_n. $g(w)$ is of the form $c|w|^2 + dw + \bar{d}\bar{w} + e$ with $c < 0$, e real, and d complex. (c is strictly negative since it is $-\det(D(z_1, \dots, z_{n-1}; w_1, \dots, w_{n-1})$ and we are supposing (6.19) and $n \geq 2$.) Thus, the set $g(w) \geq 0$ is a disk and since $g(w_n) > 0$, w_n is in its interior. Let w_0 be the center of this disk, R its radius, and let $w(\theta) = w_0 + Re^{i\theta}$. Since we have proven (1) $\Rightarrow$ (2), there is a unique Φ with

$$\Phi_\theta(z_i) = w_i, \quad i = 1, \dots, n-1; \qquad \Phi_\theta(z_n) = w(\theta) \tag{6.20}$$

and it is a rational function of degree at most $n-1$.

As usual, we can suppose $z_1 = w_1 = i$ so each $\Phi_\theta(z)$ has the form

$$\Phi_\theta(z) = \int \frac{1 + xz}{x - z}\, d\sigma_\theta(x), \tag{6.21}$$

where $d\sigma_\theta$ is a probability measure on $\mathbb{R} \cup \{\infty\}$. If $\theta_k \to \theta_\infty$, and $d\sigma_{\theta_k} \to d\rho$, then the Herglotz function associated to $d\rho$ obeys (6.20) for θ_∞ and so it must be Φ_{θ_∞}. It follows (since the probability measures are compact) that $d\rho = d\sigma_{\theta_\infty}$ and thus $\{d\sigma_\theta\}$ is closed and $d\sigma_\theta \mapsto \Phi_\theta$ is continuous. Since a continuous bijection between compact sets has a continuous inverse, $\theta \mapsto d\sigma_\theta$ is continuous.

Since Φ_θ is unique, $d\sigma_\theta$ is a pure point measure with at most $n-1$ pure points. Since the function is not determined by $(z_1, \dots, z_{n-1})$, there must be exactly $n-1$ points. It follows that the points in the support must vary continuously in θ.

Note next that for any θ, we can find θ' and $t_\theta \in (0,1)$ so that

$$w_n = t_\theta w(\theta) + (1-t_\theta) w(\theta').$$

Suppose that there is a unique Φ obeying (6.12). It follows that for any θ,

$$\Phi(z) = t_\theta \Phi_\theta(z) + (1-t_\theta)\Phi_{\theta'}(z) \tag{6.22}$$

and thus $\Phi(z)$ has a representation of the form (6.21) with $d\sigma$ a point measure with at most $2n-2$ pure points. By (6.22) again, each $d\sigma_\theta$ must be supported in that $2n-2$ point set, and then by continuity, in a fixed $n-1$ point set. But if $d\sigma_\theta$ is supported in a fixed θ-independent $n-1$ point set, so is $d\sigma$, and thus (6.19) fails. We conclude that there must be multiple Φ's obeying (6.12). $\square$

Appendix A: The Theory of Moments and Determinantal Formulae

The theory of moments has a variety of distinct objects constructed in principle from the moments $\{\gamma_n\}_{n=0}^\infty$: the orthogonal polynomials $\{P_n(x)\}_{n=0}^\infty$, the associated polynomials $\{Q_n(x)\}_{n=0}^\infty$, the sums $\sum_{j=0}^n P_j(0)^2$ and $\sum_{j=0}^n Q_j(0)^2$, the Jacobi matrix coefficients, and the approximations $-\frac{Q_n(x)}{P_n(x)}$ and $-\frac{N_n(x)}{M_n(x)}$. It turns out most of these objects can be expressed as determinants. These formulae are compact and elegant, but for some numerical applications, they suffer from numerical round-off errors in large determinants.

We have already seen two sets of determinants in Theorem 1. Namely, let $\mathcal{H}_N$ be the $N \times N$ matrix,

$$\mathcal{H}_N = \begin{pmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_{N-1} \\ \gamma_1 & \gamma_2 & \cdots & \gamma_N \\ \vdots & \vdots & & \vdots \\ \gamma_{N-1} & \gamma_N & \cdots & \gamma_{2N-2} \end{pmatrix} \tag{A.1a}$$

and $\mathcal{S}_N$, the matrix

$$\mathcal{S}_N = \begin{pmatrix} \gamma_1 & \gamma_2 & \cdots & \gamma_N \\ \gamma_2 & \gamma_3 & \cdots & \gamma_{N+1} \\ \vdots & \vdots & & \vdots \\ \gamma_N & \gamma_{N+1} & \cdots & \gamma_{2N-1} \end{pmatrix} \tag{A.1b}$$

and define

$$h_N = \det(\mathcal{H}_N), \qquad s_N = \det(\mathcal{S}_n) \tag{A.2}$$

(for comparison, D_N from [1] is our h_{N+1}). We will use $h_N(\gamma)$ if we need to emphasize what moments $\{\gamma_n\}_{n=0}^\infty$ are involved. Thus, Theorem 1 says $h_N > 0$ for all N is equivalent

to solubility of the Hamburger problem and $h_N > 0$, $s_N > 0$ for all N is equivalent to solubility of the Stieltjes problem.

There is an interesting use of determinants to rewrite h_N and s_N in terms of the moment problem that makes their positivity properties evident. Suppose $d\rho$ obeys (1.1). Then

$$\begin{aligned} h_N &= \int \det((x_a^{a+b})_{0\le a,b\le N-1}) \prod_{a=0}^{N-1} d\rho(x_a) \\ &= \int \left[\prod_{a=1}^{n} x_a^a\right] \det((x_a^b))_{0\le a,b\le N-1} \prod_{a=0}^{N-1} d\rho(x_a). \end{aligned}$$

Permuting over indices, we see that in $\prod_{a=1}^n (x_a^a)\det(x_a^b)$, we can replace x_a by $x_{\pi(a)}$ for any permutation, π. Since $\det(x_{\pi(a)}^b) = (-1)^\pi \det(x_a^b)$, we see that

$$h_N = (N!)^{-1} \int [\det((x_a^b)_{0\le a,b\le N-1})]^2 \prod_{a=0}^{N-1} d\rho(x_a).$$

Recognizing the Vandermonde determinant, we have

$$h_N = (N!)^{-1} \int \prod_{0\le a<b\le N-1} (x_a - x_b)^2 \prod_{a=0}^{N-1} d\rho(x_a). \tag{A.3a}$$

Similarly,

$$s_N = (N!)^{-1} \int x_0 \dots x_{N-1} \prod_{0\le a<b\le N-1} (x_a - x_b)^2 \prod_{a=0}^{N-1} d\rho(x_a). \tag{A.3b}$$

The most basic formula is:

Theorem A.1. *$P_n(x)$ is given by*

$$P_n(x) = \frac{1}{\sqrt{h_n h_{n+1}}} \det \begin{pmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_n \\ \gamma_1 & \gamma_2 & \cdots & \gamma_{n+1} \\ \vdots & \vdots & & \vdots \\ \gamma_{n-1} & \gamma_n & \cdots & \gamma_{2n-1} \\ 1 & x & \dots & x^n \end{pmatrix}. \tag{A.4}$$

Proof. Let $S_n(x)$ be the determinant on the right side of (A.4). Then for any solution ρ of the moment problem, we have that $\int S_n(x) x^j \, d\rho(x)$ is given by the same determinant, but with the last row replaced by $\gamma_j \; \gamma_{j+1} \; \dots \; \gamma_{j+n}$. It follows that

$$\begin{aligned} \int x^j S_n(x)\, d\rho(x) &= 0, && j = 0, 1, \dots, n-1 \\ &= h_{n+1} && j = n. \end{aligned} \tag{A.5}$$

In particular, since

$$S_n(x) = h_n x^n + \text{ lower order}, \tag{A.6}$$

we see that

$$\int S_n(x)^2\, d\rho(x) = \; h_n h_{n+1}. \tag{A.7}$$

From (A.5)–(A.7), it follows that $P_n(x) = \frac{S_n(x)}{\sqrt{h_n h_{n+1}}}$. $\square$

From (A.4), we can deduce formulae for the coefficients a_n, b_n of a Jacobi matrix associated to the moments $\{\gamma_n\}_{n=0}^{\infty}$. Let $\tilde{h}_n$ be the $n \times n$ determinant obtained by changing the last column in $\mathcal{H}_N$:

$$\tilde{h}_n = \det \begin{pmatrix} \gamma_0 & \gamma_1 & \cdots & \gamma_{n-2} & \gamma_n \\ \vdots & \vdots & & \vdots & \vdots \\ \gamma_n & \gamma_{n+1} & \cdots & \gamma_{2n-3} & \gamma_{2n-1} \end{pmatrix}.$$

Thus (A.4) implies that

$$P_n(x) = \sqrt{\frac{h_n}{h_{n+1}}} \left[x^n - \frac{\tilde{h}_n}{h_n}\, x^{n-1} + \text{ lower order} \right]. \tag{A.8}$$

Theorem A.2. *For $n \geq 0$,*

$$\text{(i)} \qquad a_n = \left(\frac{h_n h_{n+2}}{h_{n+1}^2} \right)^{1/2}$$

$$\text{(ii)} \qquad \sum_{j=0}^{n} b_j = \frac{\tilde{h}_{n+1}}{h_{n+1}}\,.$$

Proof. By the definition of a_n and b_n, we have that

$$xP_n(x) = a_n P_{n+1}(x) + b_n P_n(x) + a_{n-1} P_{n-1}(x). \tag{A.9}$$

Identifying the x^{n+1} and x^n terms in (A.9) using (A.8), we see that

$$\sqrt{\frac{h_n}{h_{n+1}}} = a_n \sqrt{\frac{h_{n+1}}{h_{n+2}}} \tag{A.10}$$

$$\sqrt{\frac{h_n}{h_{n+1}}} \left(-\frac{\tilde{h}_n}{h_n} \right) = a_n \sqrt{\frac{h_{n+1}}{h_{n+2}}} \left(-\frac{\tilde{h}_{n+1}}{h_{n+1}} \right) + b_n \sqrt{\frac{h_n}{h_{n+1}}}\,. \tag{A.11}$$

(A.10) implies (i) immediately, and given (A.10), (A.11) becomes

$$b_n = \frac{\tilde h_{n+1}}{h_{n+1}} - \frac{\tilde h_n}{h_n}\,,$$

which implies (ii) by induction if we note the starting point comes from looking at the constant term in $xP_0(x) = x = a_0P_1(x) + b_0P_0(x)$, which implies that $b_0 = \frac{\tilde h_1}{h_1} = \frac{\gamma_1}{\gamma_0}$. $\square$

Remark. (ii) has an alternate interpretation. (A.8) says that $\frac{\tilde h_{n+1}}{h_{n+1}}$ is the sum of the $n+1$ roots of $P_{n+1}(x)$. But $P_{n+1}(x)$ is a multiple of the determinant of the Jacobi matrix $A_F^{[n+1]}$. So the sum of the roots is just the trace of $A_F^{[n+1]}$, that is, $\sum_{j=0}^n b_j$.

From (A.4) and Theorem 4.2, (i.e., $Q_n(x) = E_X(\frac{P_n(X)-P_n(Y)}{X-Y})$), we immediately get

Theorem A.3.

$$Q_n(x) = \frac{1}{\sqrt{h_nh_{n+1}}}\det\begin{pmatrix} \gamma_0 & \gamma_1 & \dots & \gamma_n \\ \gamma_1 & \gamma_2 & \dots & \gamma_{n+1} \\ \vdots & \vdots & & \vdots \\ \gamma_{n-1} & \gamma_n & \dots & \gamma_{2n-1} \\ R_{n,0}(x) & R_{n,1}(x) & \dots & R_{n,n}(x) \end{pmatrix} \tag{A.12}$$

where

$$R_{n,j}(x) = \sum_{k=0}^{j-1} \gamma_{j-1-k}x^k, \qquad j \geq 1 \tag{A.13a}$$

$$R_{n,j=0}(x) = 0. \tag{A.13b}$$

Proof. $\frac{x^j-y^j}{x-y} = \sum_{k=0}^{j-1} y^{j-1-k}x^k$ so $E_X(\frac{x^j-y^j}{x-y}) = R_{n,j}(x)$. $\square$

Remark. By (A.4), $P_n(x)\sum_{k=0}^{2n-1}\gamma_kx^{-k-1}$ has the same form as (A.4) but with the bottom row replaced by $S_{n,0}(x)\dots S_{n,n}(x)$ where

$$\begin{aligned} S_{n,j}(x) &= \sum_{k=0}^{2n-1}\gamma_kx^{j-k-1} = \sum_{\ell=-(2n-j)}^{j-1}\gamma_{j-1-\ell}x^\ell \\ &= R_{n,j}(x) + x^{-1}\gamma_j + x^{-2}\gamma_{j+1} + \dots + x^{-n}\gamma_{j+n-1} + O(x^{-n-1}). \end{aligned}$$

Recognizing $x^{-1}\gamma_j + x^{-2}\gamma_{j+1} + \dots + x^{-n-1}\gamma_{j+n-1}$ as x^{-1} times the first row of the matrix in (A.4) plus x^{-2} times the second row plus ..., we conclude that

$$P_n(x)\biggl(\sum_{k=0}^{2n-1}\gamma_kx^{-k-1}\biggr) = Q_n(x) + O(x^{-n-1})$$

and thus

$$-\frac{Q_n(x)}{P_n(x)} = -\sum_{k=0}^{2n-1}\gamma_kx^{-k-1} + O(x^{-2n-1})$$

consistent with the $f^{[N-1,N]}$ Padé formula (5.28).

We saw the quantity L of (5.29) is important. Here is a formula for it.

Theorem A.4. *$L = \lim_{n\to\infty} -\frac{Q_n(0)}{P_n(0)}$ and*

$$-\frac{Q_n(0)}{P_n(0)} = \frac{t_n}{s_n}\,, \tag{A.14a}$$

where $s_n = \det(\mathcal{S}_N)$ and

$$t_n = -\det\begin{pmatrix} 0 & \gamma_0 & \gamma_1 & \dots & \gamma_n \\ \gamma_0 & \gamma_1 & \gamma_2 & \dots & \gamma_{2n+1} \\ \vdots & \vdots & \vdots & & \vdots \\ \gamma_n & \gamma_{n+1} & \gamma_{n+2} & \dots & \gamma_{2n-1} \end{pmatrix}. \tag{A.14b}$$

Proof. Follows by putting $x = 0$ in our formula for $P_n(x)$ and $Q_n(x)$. $\square$

Next we have explicit formulae for $M_n(x)$ and $N_n(x)$, the polynomials introduced for Section 5 (see (5.15) and (5.16)).

Theorem A.5.

$$M_n(x) = \frac{1}{s_{n-1}}\sqrt{\frac{h_n}{h_{n+1}}}\begin{pmatrix} \gamma_1 & \gamma_2 & \dots & \gamma_n \\ \gamma_2 & \gamma_3 & \dots & \gamma_{n+1} \\ \vdots & \vdots & & \vdots \\ \gamma_{n-1} & \gamma_{n-2} & \dots & \gamma_{2n-2} \\ x & x^2 & \dots & x^n \end{pmatrix} \tag{A.15}$$

$$N_n(x) = \frac{1}{s_{n-1}}\sqrt{\frac{h_n}{h_{n+1}}}\begin{pmatrix} \gamma_1 & \gamma_2 & \dots & \gamma_n \\ \gamma_2 & \gamma_3 & \dots & \gamma_{n+1} \\ \vdots & \vdots & & \vdots \\ \gamma_{n-1} & \gamma_{n-2} & \dots & \gamma_{2n-2} \\ R_{n,1}(x) & R_{n,2}(x) & \dots & R_{n,n}(x) \end{pmatrix} \tag{A.16}$$

where $R_{i,j}(x)$ is given by (A.13).

Remarks. 1. P_n is given by a $(n+1)\times(n+1)$ matrix. To get M_n, which has an $n\times n$ matrix, we drop the first column and next to last row.

2. It is interesting that (A.15) does not obviously follow from the basic definition (5.15).

Proof. The right side of (A.15) (call it $\widetilde{M}_n(x)$) has the following properties:

(i) It is a polynomial of degree n.
(2) It obeys $\widetilde{M}_n(0) = 0$.
(3) It obeys $E_x(x^j\widetilde{M}_n(x)) = 0$ for $j = 0, 1, \dots, n-2$ since the corresponding matrix has two equal rows.
(4) It obeys $\widetilde{M}_n(x) = \sqrt{h_n/h_{n+1}}\, x^n +$ lower order so it has the same highest degree term as $P_n(x)$.

These properties uniquely determine $M_n(x)$ so (A.15) is proven. (A.16) then follows from (5.24). $\square$

Remark. By mimicking the argument following Theorem A.3, one finds that

$$M_n(x) \sum_{k=0}^{2n-2} \gamma_k x^{-k-1} = N_n(x) + O(x^{-n})$$

so that

$$-\frac{N_n(x)}{M_n(x)} = -\sum_{k=0}^{2n-2} \gamma_k x^{-k-1} + O(x^{-2n}),$$

consistent with the $f^{[N-1,N-1]}$ Padé formula used in the proof of Theorem 6 (at the end of Section 5).

Remarkably, there are also single determinant formulae for $\sum_{j=0}^{n} P_j(0)^2$ and $\sum_{j=0}^{n} Q_j(0)^2$.

Theorem A.6. *We have that*

$$\sum_{j=0}^{n} P_j(0)^2 = \frac{v_n}{h_{n+1}} \tag{A.17}$$

$$\sum_{j=0}^{n} Q_j(0)^2 = -\frac{w_{n+2}}{h_{n+1}}, \tag{A.18}$$

where v_n is given by the $n \times n$ determinant,

$$v_n = \det \begin{pmatrix} \gamma_2 & \cdots & \gamma_{n+1} \\ \gamma_3 & \cdots & \gamma_{n+2} \\ \vdots & & \vdots \\ \gamma_{n+1} & \cdots & \gamma_{2n} \end{pmatrix} \tag{A.19}$$

and w_{n+2} by the $(n+2) \times (n+2)$ determinant,

$$w_n = \det \begin{pmatrix} 0 & 0 & \gamma_0 & \gamma_1 & \cdots & \gamma_{n-1} \\ 0 & \gamma_0 & \gamma_1 & \gamma_2 & \cdots & \gamma_n \\ \gamma_0 & \gamma_1 & \gamma_2 & \gamma_3 & \cdots & \gamma_{n+1} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ \gamma_{n-1} & \gamma_n & \gamma_{n+1} & \gamma_{n+2} & \cdots & \gamma_{2n} \end{pmatrix} \tag{A.20}$$

Remark. Thus by Theorems 3 and 7, indeterminacy for both the Hamburger and Stieltjes problems can be expressed in terms of limits of ratios of determinants. In the Hamburger

case, we need (A.17) and (A.18) to have finite limits in order that the problem be indeterminate. In the Stieltjes case, (A.17) and (A.14) must have finite limits for indeterminacy to hold.

Proof. We actually prove a stronger formula. Let

$$B_N(x,y) = \sum_{n=0}^{N} P_n(x)P_n(y). \tag{A.21}$$

We will show that

$$B_n(x,y) = -h_{n+1}^{-1} \det \begin{pmatrix} 0 & 1 & x & \dots & x^N \\ 1 & \gamma_0 & \gamma_1 & \dots & \gamma_N \\ y & \gamma_1 & \gamma_2 & \dots & \gamma_{N+1} \\ \vdots & \vdots & \vdots & & \vdots \\ y^N & \gamma_N & \gamma_{N+1} & \dots & \gamma_{2N} \end{pmatrix} \tag{A.22}$$

(A.17) then follows by setting $x = y = 0$ and noting that if $C = \{C_{ij}\}_{1\le i\le j\le N}$ is an $N\times N$ matrix with $C_{11} = 0$, $C_{1j} = \delta_{2j}$, and $C_{i1} = \delta_{i2}$, then

$$\det((C_{ij})_{1\le i,j\le N}) = -\det((C_{ij})_{3\le i,j\le N}).$$

(A.18) then follows from $Q_j(z) = E_x\bigl(\frac{[P_j(x)-P_j(z)]}{(x-z)}\bigr)$, since

$$\sum_{n=0}^{N} Q_n(0)^2 = E_xE_y([B_N(x,y) - B_N(x,0) - B_N(0,y) + B_N(0,0)]x^{-1}y^{-1}).$$

Thus we need only prove (A.22). To do this, let $\tilde{B}_N(x,y)$ be the right side of (A.22). Consider $E_x(\tilde{B}_N(x,y)x^j)$ for $0\le j\le N$. This replaces the top row in the determinant by $(0\ \gamma_j\ \gamma_{j+1}\ \dots\ \gamma_{N+j})$. The determinant is unchanged if we subtract the row $(y^j\ \gamma_j\ \dots\ \gamma_{N+j})$ from this row. That is, $E_x(\tilde{B}_N(x,y)x^j)$ is given by the determinant with top row $(-y^j\ 0\ 0\ \dots\ 0)$. Thus,

$$E_x(\tilde{B}_N(x,y)x^j) = -h_{n+1}^{-1}(-y^j)h_{n+1} = y^j.$$

So, $\tilde{B}_N(x,y)$ is a reproducing kernel. For any polynomial $P(x)$ of degree N or smaller, $E_x(\tilde{B}_N(x,y)P(x)) = P(y)$. But

$$\tilde{B}_N(x,y) = \sum_{j=0}^{N} E_x(\tilde{B}_N(x,y)P_j(x))P_j(x) = B_N(x,y)$$

since $\{P_j(x)\}_{j=0}^N$ is an orthonormal basis in the polynomials of degree N or less. Thus (A.22) is proven. □

In terms of the $\gamma^{(\ell)}$ moment problems (with moments $\gamma_j^{(\ell)} = \frac{\gamma_{\ell+j}}{\gamma_\ell}$), we recognize v_n as $(\gamma_2)^{n-1} h_{n-1}(\gamma^{(2)})$. By (A.17) for the $\gamma^{(2)}$ problem,

$$\sum_{j=0}^{n-1} P_j^{(2)}(0) = \frac{v_{n-1}(\gamma^{(2)})}{h_n(\gamma^{(2)})}\,.$$

But $h_n(\gamma^{(2)}) = v_n(\gamma)(\gamma_2)^{-n}$ and $v_{n-1}(\gamma^{(2)}) = \gamma_2^{1-n} y_{n-1}(\gamma)$ where

$$y_{n-1} = \begin{pmatrix} \gamma_4 & \cdots & \gamma_{n+2} \\ \gamma_5 & \cdots & \gamma_{n+3} \\ \vdots & & \vdots \\ \gamma_{n+1} & \cdots & \gamma_{2n} \end{pmatrix}. \tag{A.23}$$

Thus, using Proposition 5.13:

Theorem A.7.

$$\gamma_2^{-1}\biggl(\sum_{j=0}^{n} P_j(0)^2\biggr)\biggl(\sum_{j=0}^{n-1} P_j^{(2)}(0)^2\biggr) = \frac{y_{n-1}}{h_{n+1}}\,.$$

In particular, the Hamburger problem is determinate if and only if $\lim_{n\to\infty} \frac{y_{n-1}}{h_{n+1}} = \infty$.

So we have a simple ratio of determinants to determine determinacy.

Appendix B: The Set of Solutions of the Moment Problem as a Compact Convex Set

In this appendix, we will prove (following [1]) that $\mathcal{M}^H(\gamma)$ and $\mathcal{M}^S(\gamma)$ are compact convex sets whose extreme points are dense. Each set is a subset of $\mathcal{M}_+(\mathbb{R}\cup\{\infty\})$, the set of measures on the compact set $\mathbb{R}\cup\{\infty\}$. This set, with the condition $\int d\rho(x) = \gamma_0$, is a compact space in the topology of weak convergence (i.e., $\int f(x)\,d\rho_n(x) \to \int f(x)\,d\rho(x)$ for continuous functions f on $\mathbb{R}\cup\{\infty\}$).

Theorem B.1. *$\mathcal{M}^H(\gamma)$ and $\mathcal{M}^S(\gamma)$ are closed in the weak topology and so are compact convex sets.*

Remark. Since the x^n's are unbounded, this does not follow from the definition of the topology without some additional argument.

Proof. By Propositions 4.4 and 4.13, $\mu \in \mathcal{M}^H(\gamma)$ if and only if

$$\int (x-z_0)^{-1}\,d\mu(x) \in D(z_0) \tag{B.1}$$

for all $z_0 \in \mathbb{C}$. The set of μ's that obey (B.1) for a fixed z_0 is closed since $D(z_0)$ is closed and $(x-z_0)^{-1}$ is in $C(\mathbb{R}\cup\{\infty\})$. Thus, the intersection over all z_0 is closed.

$\mathcal{M}^S(\gamma) = \mathcal{M}^H(\gamma) \cap \{\mu \mid \int f(x)\,d\mu(x) = 0 \text{ if } \operatorname{supp} f \subset (-\infty, 0)\}$ is an intersection of closed sets. $\square$

Remark. To get compact sets of measures, we need to consider $\mathbb{R} \cup \{\infty\}$ rather than $\mathbb{R}$. Thus a priori, the integral in (B.1) could have a point at infinity giving a constant term as $z_0 = iy$ with $y \to \infty$. Since $D(z_0) \to \{0\}$ as $z_0 = iy$ with $y \to \infty$, this term is absent.

Theorem B.2 (Naimark). *$\mu \in \mathcal{M}^H(\gamma)$ (resp. $\mathcal{M}^S(\gamma)$) is an extreme point if and only if the polynomials are dense in $L^1(\mathbb{R}, d\rho)$.*

Remark. Compare with density in $L^2(\mathbb{R}, d\rho)$ which picks out the von Neumann solutions.

Proof. This is a simple use of duality theory. The polynomials fail to be dense if and only if there exists a non-zero $F \in L^\infty(\mathbb{R}, d\rho)$ so that

$$\int x^n F(x)\,d\rho(x) = 0 \tag{B.2}$$

for all n. We can suppose that $\|F\|_\infty = 1$, in which case $d\rho_\pm = (1 \pm F)\,d\rho$ both lie in $\mathcal{M}^H(\gamma)$ with $\rho = \frac{1}{2}(\rho_+ + \rho_-)$, so ρ is not extreme.

Conversely, suppose $\rho = \frac{1}{2}(\rho_+ + \rho_-)$ with $\rho_+ \neq \rho_-$ and both in $\mathcal{M}^H(\gamma)$. Then $\rho_\pm \leq 2\rho$ so ρ_+ is ρ-absolutely continuous, and the Radon-Nikodyn derivative, $\frac{d\rho_+}{d\rho}$, obeys $\|\frac{d\rho_+}{d\rho}\|_\infty \leq 2$. Let $F = 1 - \frac{d\rho_+}{d\rho}$, so $\|F\|_\infty \leq 1$ and $F \neq 0$ since $\rho_+ \neq \rho_-$. Then

$$\int F(x) x^n\,d\rho = \int x^n\,d\rho - \int x^n\,d\rho_+ = 0.$$

Thus, we have proven the result for $\mathcal{M}^H(\gamma)$. Since $\mathcal{M}^S(\gamma) = \{\rho \in \mathcal{M}^H(\gamma) \mid \int f(x)\,d\rho(x) = 0 \text{ for } f \text{ in } C(\mathbb{R} \cup \{\infty\}) \text{ with support in } (-\infty, 0)\}$, $\mathcal{M}^S(\gamma)$ is a face of $\mathcal{M}^H(\gamma)$, so extreme points of $\mathcal{M}^S(\gamma)$ are exactly those extreme points of $\mathcal{M}^H(\gamma)$ that lie in $\mathcal{M}^S(\gamma)$. $\square$

Theorem B.3. *Let $\rho \in \mathcal{M}^H(\gamma)$ have $\operatorname{ord}(\rho) < \infty$. Then ρ is an extreme point.*

Proof. By Theorem 6.4, for some $z_1, \dots, z_n \in \mathbb{C}_+$, we have that the polynomials are dense in $L^2(\mathbb{R}, \prod_{j+1}^n |x - z_j|^{-2} d\rho)$. For any polynomially bounded continuous function

$$\int |f(x)|\,d\rho(x) \leq \left(\int |f(x)|^2 \prod_{j=1}^n |x - z_j|^{-2}\,d\rho(x)\right)^{1/2} \left(\int \prod_{j=1}^n (x - z_j)^2\,d\rho(x)\right)^{1/2}$$

by the Schwarz inequality. It follows that the identification map is continuous from $L^2(\mathbb{R}, \prod_{j=1}^n (x - z)^{-2}\,d\rho)$ into $L^1(\mathbb{R}, d\rho)$, so the polynomials are dense in L^1-norm in the continuous functions, and so in $L^1(\mathbb{R}, d\rho)$. By Theorem B.2, ρ is an extreme point. $\square$

Theorem B.4. *The extreme points are dense in $\mathcal{M}^H(\gamma)$ (and in $\mathcal{M}^S(\gamma)$).*

Proof. The finite point measures are dense in the finite measures on $\mathbb{R}\cup\{\infty\}$. Thus, by the Herglotz representation theorem in form (6.8), if Φ is a Herglotz function, there exist real rational Herglotz functions Φ_n so that $\Phi_n(z)\to\Phi(z)$ for each $z\in\mathbb{C}_+$.

Now let $\rho\in\mathcal{M}^H(\gamma)$ and let Φ_ρ be the Nevanlinna function of ρ. Let Φ_n be as above and $\rho_n=\rho_{\Phi_n}$. Then by (4.35), $G_{\rho_n}(z)\to G_\rho(z)$ for each $z\in\mathbb{C}_+$ and so $\rho_n\to\rho$ weakly. By Theorems 6.4 and B.3, each such ρ_n is an extreme point.

For the Stieltjes case, we need only note that by Theorem 4.18 and the remark after it, if $\rho\in\mathcal{M}^S(\gamma)$, then the approximating Φ_n's can be chosen so that $\rho_{\Phi_n}\in\mathcal{M}^S(\gamma)$. □

Theorem B.5. *For any indeterminate set of Hamburger moments $\{\gamma_n\}_{n=0}^\infty$, $\mathcal{M}^H(\gamma)$ has extreme points ρ with* $\mathrm{ord}(\rho)=\infty$.

Proof. We first pick positive α_j strictly decreasing so that for any $\rho\in\mathcal{M}^H(\gamma)$ we have that

$$\sup_n \int \prod_{j=1}^n (1+\alpha_j^2x^2)^2\,d\rho(x)\le 2. \tag{B.3}$$

We can certainly do this as follows: Since the integral only depends on the moments γ_j, we need only do it for some fixed $\rho_0\in\mathcal{M}^H(\gamma)$. Since

$$\lim_{\alpha_1\downarrow 0}\int (1+\alpha_1^2x^2)^2\,d\rho(x)=1,$$

we can pick $\alpha_1>0$ so

$$\int (1+\alpha_1^2x^2)^2\,d\rho(x)<2.$$

We then pick $\alpha_2,\alpha_3,\dots$ inductively so the integral is strictly less than 2. Then the sup in (B.3) is bounded by 2. The product must be finite for a.e. x w.r.t. $d\rho$, so

$$\sum_{j=1}^\infty \alpha_j^2<\infty. \tag{B.4}$$

So if

$$g_n(x)=\prod_{j=1}^n (1+\alpha_j^2x^2),$$

then for any real x,

$$g(x)=\lim_{n\to\infty} g_n(x)$$

exists, and by (B.3),

$$\int g(x)^2\,d\rho(x)<\infty$$

for any $\rho\in\mathcal{M}^H(\gamma)$.

Now pick $\zeta_1, \zeta_2, \dots$ in $\mathbb{C}_+$ and $\rho_1, \rho_2, \dots$ in $\mathcal{M}^H(\gamma)$ inductively so ρ_k obeys

$$\int (x - i\alpha_j^{-1})^{-1}\, d\rho_k(x) = \zeta_j, \qquad j = 1, \dots, k \tag{B.5}$$

and then ζ_{k+1} is the middle of the disk of allowed values for $\int (x - i\alpha_{j+1}^{-1})^{-1}\, d\rho(x)$ for those ρ in $\mathcal{M}^H(\gamma)$ which obey (B.5). Pick a subsequence of the ρ_j's which converges to some $\rho_\infty \in \mathcal{M}^H(\gamma)$. Then ρ_∞ obeys (B.5) for all k.

Let

$$\mathcal{M}_k = \{\rho \in \mathcal{M}^H(\gamma) \mid \rho \text{ obeys (B.5)}\}$$

and

$$\mathcal{M}_\infty = \cap \mathcal{M}_k.$$

Define for all n, m,

$$\Gamma_m^{(n)} = \int x^m \prod_{j=1}^n (1 + \alpha_j^2 x^2)^{-1}\, d\rho_n(x).$$

By Theorem 6.1, $\mu \in \mathcal{M}^H(\Gamma^{(n)})$ if and only if $d\rho \equiv g_n\, d\mu$ lies in $\mathcal{M}_k$. $\Gamma_m^{(n)}$ is decreasing to $\Gamma_m^{(\infty)}$ and

$$\Gamma_m^{(\infty)} = \int x^m g(x)^{-1}\, d\rho(x)$$

by a simple use of the monotone convergence theorem.

We claim that $\mu \in \mathcal{M}^H(\Gamma^{(\infty)})$ if and only if $d\rho = g\, d\mu$ lies in $\mathcal{M}_\infty$. For

$$\gamma_n = \lim_{n\to\infty} \int x^m g(x)^{-1} g_n(x)\, d\rho(x)$$

and the right side only depends on the moments $\Gamma_m^{(\infty)}$ and similarly for calculation of $\int (x - i\alpha_j)^{-1}\, d\rho(x)$.

Now let μ be a von Neumann solution of the $\Gamma^{(\infty)}$ moment problem and $d\rho = g\, d\mu$. Since $\int g^2\, d\rho < \infty$ by construction, the proof of Theorem B.3 shows that ρ is an extreme point. On the other hand, since ρ obeys (B.5) and ζ_j is not in the boundary of its allowed circle, $\text{ord}(\rho) = \infty$. $\square$

Appendix C: Summary of Notation and Constructions

Since there are so many objects and constructions associated to the moment problem, I am providing the reader with this summary of them and where they are discussed in this paper.

C1 Structure of the Set of Moments.

$\{\gamma_n\}_{n=0}^{\infty}$ is called a set of *Hamburger moments* if there is a positive measure ρ on $(-\infty,\infty)$ with $\gamma_n = \int x^n\, d\rho(x)$ and a set of *Stieltjes moments* if there is a ρ with support in $[0,\infty)$. We take $\gamma_0 = 1$ and demand $\operatorname{supp}(\rho)$ is not a finite set. Theorem 1 gives necessary and sufficient conditions for existence. If there is a unique ρ, the problem is called *determinate*. If there are multiple ρ's, the problem is called *indeterminate*. If a set of Stieltjes moments is Hamburger determinate, it is a fortiori Stieltjes determinate. But the converse can be false (see the end of Section 3).

$\mathcal{M}^H(\gamma)$ (resp. $\mathcal{M}^S(\gamma)$) denotes the set of all solutions of the Hamburger problem (resp. all $\rho \in \mathcal{M}^H(\gamma)$ supported on $[0,\infty)$). They are compact convex sets (Theorem B.1) whose extreme points are dense (Theorem B.4). Indeterminate Hamburger problems have a distinguished class of solutions we have called *von Neumann solutions* (called N-extremal in [1] and extremal in [35]). They are characterized as those $\rho \in \mathcal{M}^H(\gamma)$ with the polynomials dense in $L^2(\mathbb{R}, d\rho)$. They are associated to self-adjoint extensions B_t of the Jacobi matrix associated to γ (see **C4** below for the definition of this Jacobi matrix). The parameter t lies in $\mathbb{R} \cup \{\infty\}$ and is related to B_t and the solution $\mu_t \in \mathcal{M}^H(\gamma)$ by

$$t = (\delta_0, B_t^{-1}\delta_0) = \int x^{-1} d\mu_t(x). \tag{C.1}$$

In the indeterminate Stieltjes case, there are two distinguished solutions: μ_F, the *Friedrichs solution*, and μ_K, the *Krein solution*. Both are von Neumann solutions of the associated Hamburger problem and are characterized by $\inf[\operatorname{supp}(\mu_F)] > \inf[\operatorname{supp}\rho]$ for any other $\rho \in \mathcal{M}^H(\gamma)$ and by $\mu_K(\{0\}) > 0$ and $\mu_K(\{0\}) > \rho(\{0\})$ for any other $\rho \in \mathcal{M}^H(\gamma)$ (see Theorems 3.2 and 4.11 and 4.17). All solutions of the Stieltjes problem lie between μ_F and μ_K in the sense of (4.42) (see Theorem 5.10).

We define

$$\mathbb{C}_+ = \{z \in \mathbb{C} \mid \operatorname{Im} z > 0\}.$$

For any probability measure ρ, we define its *Stieltjes transform* as a function of $\mathbb{C}\backslash\operatorname{supp}(\rho)$ by

$$G_\rho(z) = \int \frac{d\rho(x)}{x - z}\,.$$

These functions map $\mathbb{C}_+$ to $\mathbb{C}_+$ and have an asymptotic series

$$G_\rho(z) \sim -z^{-1}\left(\sum_{j=0}^{\infty} \gamma_j z^{-j}\right) \tag{C.2}$$

as $|z| \to \infty$ with $\min(|\operatorname{Arg}(z)|, |\operatorname{Arg}(-z)|) > \varepsilon$. (C.2) characterizes $\mathcal{M}^H(\gamma)$ and the asymptotics are uniform over $\mathcal{M}^H(\gamma)$ (Proposition 4.13).

For an indeterminate moment problem, we defined $\operatorname{ord}(\rho)$, the *order* of ρ, to be the codimension of the closure of the polynomials in $L^2(\mathbb{R}, d\rho)$. The solutions of finite order are dense in $\mathcal{M}^H(\gamma)$ and in $\mathcal{M}^S(\gamma)$, and each is an extreme point. Solutions of finite

order (and, in particular, the von Neumann solutions) are discrete pure point measures; equivalently, their Stieltjes transforms are meromorphic functions (Theorems 4.11 and 6.4).

C2 Nevanlinna Parametrization.

We used $\mathcal{F}$ to denote the analytic maps of $\mathbb{C}_+$ to $\bar{\mathbb{C}}_+$ where the closure is in the Riemann sphere. The open mapping theorem implies that if $\Phi \in \mathcal{F}$, either $\Phi(z) \equiv t$ for some $t \in \mathbb{R} \cup \{\infty\}$ or else Φ is a Herglotz function which has a representation of the form (1.19).

Associated to any indeterminate moment problem are four entire functions, $A(z)$, $B(z)$, $C(z)$, $D(z)$, obeying growth condition of the form $|f(z)| \leq c_\varepsilon \exp(\varepsilon|z|)$. We defined them via the transfer matrix relation (4.16), but they also have explicit formulae in terms of the orthogonal polynomials, P and Q (defined in **C4** below)—these are given by Theorem 4.9.

We define a fractional linear transformation $F(z) : \mathbb{C} \cup \{\infty\} \to \mathbb{C} \cup \{\infty\}$ by

$$F(z)(w) = -\frac{C(z)w + A(z)}{D(z)w + B(z)}\,. \tag{C.3}$$

For indeterminate Hamburger problems, there is a one-one correspondence between $\rho \in \mathcal{M}^H(\gamma)$ and $\Phi \in \mathcal{F}$ given by

$$G_\rho(z) = F(z)(\Phi(z)) = -\frac{C(z)\Phi(z) + A(z)}{D(z)\Phi(z) + B(z)} \tag{C.4}$$

for $z \in \mathbb{C}_+$ (Theorem 4.14). Φ is called the Nevanlinna function of ρ, denoted by Φ_ρ. The von Neumann solutions correspond precisely to $\Phi(z) = t$ where t is given by (C.1) (Theorem 4.10). The solutions of finite order correspond precisely to the case where Φ is a ratio of real polynomials (Theorem 6.4).

Given a set of Stieltjes moments, the $\rho \in \mathcal{M}^S(\gamma)$ are precisely those $\rho \in \mathcal{M}^H(\gamma)$ whose Nevanlinna function has the form (Theorem 4.18)

$$\Phi(z) = d_0 + \int_0^\infty \frac{d\mu(x)}{x - z}$$

with $\int d\mu(x) < \infty$ and $d_0 \geq t_F = \int d\rho_F(x) = (\delta_0, A_F^{-1}\delta_0)$.

For $z \in \mathbb{C}_+$, the image of $\bar{\mathbb{C}}_+ \cup \{\infty\}$ under $F(z)$ is a closed disk denoted by $\mathcal{D}(z)$. Von Neumann solutions ρ have $G_\rho(z) \in \partial\mathcal{D}(z)$ for all z while other solutions have $G_\rho(z) \in \mathcal{D}(z)^{\text{int}}$ for all z (Theorem 4.3, Proposition 4.4, and Theorem 4.14).

C3 Derived Moment Problems.

Any set of moments has many families of associated moments. For each real c, $\gamma(c)$ is defined by

$$\gamma_n(c) = \sum_{j=0}^{n} \binom{n}{j} c^j \gamma_{n-j}. \tag{C.5}$$

There is a simple map ($\rho \mapsto \rho(\,\cdot\, - c)$) that sets up a bijection between $\mathcal{M}^H(\gamma)$ and $\mathcal{M}^H(\gamma(c))$ and, in particular, γ is Hamburger determinate if and only if $\gamma(c)$ is Hamburger determinate. But the analog is not true for the Stieljes problem. Indeed, (end of Section 3), if γ is a set of indeterminate Stieltjes moments and $c_F = -\inf \operatorname{supp}(d\mu_F)$, then $\gamma(c)$ is a set of Stieltjes moments if and only if $c \geq c_F$, and it is Stieltjes determinate if and only if $c = c_F$. The orthogonal polynomials for $\gamma(c)$ and γ are related via $P_N^{(\gamma(c))}(z) = P_N(z-c)$.

Given a set of Stieltjes moments $\{\gamma_n\}_{n=0}^\infty$, one defines Hamburger moments $\{\Gamma_n\}_{n=0}^\infty$ by

$$\Gamma_{2m} = \gamma_m, \qquad \Gamma_{2m+1} = 0. \tag{C.6}$$

There is a simple map ($d\rho \mapsto d\mu(x) = \frac{1}{2}\chi_{[0,\infty)}(x)\, d\rho(x^2) + \frac{1}{2}\chi_{(-\infty,0]}(x)\, d\rho(x^2)$) that sets up a bijection between $\mathcal{M}^H(\gamma)$ and those $\mu \in \mathcal{M}^H(\Gamma)$ with $d\mu(-x) = d\mu(x)$. Then γ is Stieltjes determinate if and only if the Γ problem is Hamburger determinate (Theorem 2.13). There are simple relations between the orthogonal polynomials for γ and those for Γ ((5.89)–(5.92)).

For $\ell = 1, 2, \dots$, define

$$\gamma_j^{(\ell)} = \frac{\gamma_{\ell+j}}{\gamma_\ell}\,. \tag{C.7}$$

If γ is a set of Stieltjes moments, so are $\gamma^{(\ell)}$ for all ℓ, and if γ is a set of Hamburger moments, so are $\gamma^{(\ell)}$ for $\ell = 2, 4, \dots$. The map $\rho \mapsto d\rho^{(\ell)} = x^\ell \frac{d\rho(x)}{\gamma_\ell}$ is a map from $\mathcal{M}^H(\gamma)$ to $\mathcal{M}^H(\gamma^{(\ell)})$ which is injective. But in the indeterminate case, it is *not*, in general, surjective. If γ is indeterminate, so is $\gamma^{(\ell)}$, but the converse may be false for either the Hamburger or Stieltjes problems (Corollary 4.21). For general ℓ, the connection between the orthogonal polynomials for γ and $\gamma^{(\ell)}$ is complicated (see the proof of Proposition 5.13 for $\ell = 2$), but (see the remarks following Theorem 5.14)

$$P_N^{(1)}(z) = \frac{d_N[P_N(0)P_{N+1}(z) - P_{N+1}(0)P_N(z)]}{z}\,.$$

Given a set of Hamburger moments $\{\gamma_j\}_{j=0}^\infty$, one defines a new set $\{\gamma_j^{(0)}\}_{j=0}^\infty$ by the following formal power series relation:

$$\left[\sum_{n=0}^{\infty}(-1)^n \gamma_n z^n\right]^{-1} = 1 - \gamma_1 z + (\gamma_2 - \gamma_1^2) z^2 \left(\sum_{n=0}^{\infty} (-1)^n \gamma_n^{(0)} z^n\right). \tag{C.8}$$

This complicated formula is simple at the level of Jacobi matrices. If $\{a_n\}_{a=0}^\infty$, $\{b_n\}_{n=0}^\infty$ (resp. $\{a_n^{(0)}\}_{n=0}^\infty$, $\{b_n^{(0)}\}_{n=0}^\infty$) are the Jacobi matrix coefficients associated to γ (resp. $\gamma^{(0)}$), then

$$a_n^{(0)} = a_{n+1}, \qquad b_n^{(0)} = b_{n+1}.$$

The map $\rho \mapsto \tilde{\rho}$ given by (5.53) sets up a bijection between $\mathcal{M}^H(\gamma)$ and $\mathcal{M}^H(\gamma^{(0)})$, and, in particular, γ is a Hamburger determinate if and only if $\gamma^{(0)}$ is (Proposition 5.15). This is not, in general, true in the Stieltjes case (see Proposition 5.17). There is a simple relation between the orthogonal polynomials for γ and for $\gamma^{(0)}$; see Proposition 5.16. In particular,

$$P_N^{(0)}(z) = a_0 Q_{N+1}(z). \tag{C.9}$$

For $\ell = -1, -2, \dots$, we defined

$$\gamma^{(\ell)} = (\gamma^{(0)})^{(-\ell)} = \frac{\gamma_{j-\ell}^{(0)}}{\gamma_{-\ell}^{(0)}}\,. \tag{C.10}$$

C4 Associated Polynomials.

Given a set of Hamburger moments, the fundamental orthogonal polynomials $P_N(z)$ are defined by requiring for any $\rho \in \mathcal{M}^H(\gamma)$ that

$$\int P_j(x) P_\ell(x)\, d\rho(x) = \delta_{j\ell} \tag{C.11}$$

and $P_N(x) = c_{NN} x^N +$ lower order terms with $c_{NN} > 0$. They obey a three-term recursion relation

$$xP_N(x) = a_N P_{N+1}(x) + b_N P_N(x) + a_{N-1} P_{N-1}(x). \tag{C.12}$$

The Jacobi matrix A associated to γ is the tridiagonal matrix given by (1.16).

The associated polynomials $Q_N(x)$ are of degree $N-1$ and defined to obey (C.12) but with the starting conditions, $Q_0(x) = 0$, $Q_1(x) = \frac{1}{a_0}$. They are related to P_N by (Theorem 4.2)

$$Q_N(x) = \int \frac{P_N(x) - P_N(y)}{x-y}\, d\rho(y) \tag{C.13}$$

for any $\rho \in \mathcal{M}^H(\gamma)$. As noted in (C.9), they are up to constants, orthogonal polynomials for another moment problem, namely, $\gamma^{(0)}$.

In the Stieltjes case, we defined polynomials M_N by

$$M_N(x) = P_N(x) - \frac{P_N(0) P_{N-1}(x)}{P_{N-1}(0)}\,. \tag{C.14}$$

They vanish at $x = 0$ so $\frac{M_N(x)}{x}$ is also a polynomial. It is of degree $N-1$ and is up to a constant, the principal orthogonal polynomial of the moment problem $\gamma^{(1)}$. $N_N(x)$ is defined analogously to (C.13) with P_N replaced by M_N. In Section 5, it was useful to change the normalizations and define multiples of $P_N(-x)$, $Q_N(-x)$, $M_N(-x)$, and $N_N(-x)$ as functions $U_N(x)$, $V_N(x)$, $G_N(x)$, $H_N(x)$ given by (5.71)–(5.74).

C5 Padé Approximants and Finite Matrix Approximations.

If $\{\gamma_n\}_{n=0}^{\infty}$ is a set of Hamburger (resp. Stieltjes) moments, the formal power series $\sum_{n=0}^{\infty}(-1)^n\gamma_n z^n$ is called a *series of Hamburger* (resp. *a series of Stieltjes*). Formally, it sums to

$$\int \frac{d\rho(x)}{1+xz}$$

if $\rho \in \mathcal{M}^H(\gamma)$. The Padé approximants $f^{[N,M]}(z)$ to these series, if they exist, are defined by (5.25)–(5.27) as the rational function which is a ratio of a polynomial of degree N to a polynomial of degree M, whose first $N+M+1$ Taylor coefficients are $\{(-1)^n\gamma_n\}_{n=0}^{N+M}$.

For a series of Stieltjes, for each fixed $\ell = 0, \pm 1, \dots,$

$$\lim_{N\to\infty} f^{[N+\ell-1,N]}(z) \equiv f_\ell(z)$$

exists for all $z \in \mathbb{C}\backslash(-\infty, 0)$ and defines a function analytic there. Indeed, for $x \in [0,\infty)$, $(-1)^\ell f^{[N+\ell-1,N]}(x)$ is monotone increasing (Theorem 6, Theorem 5.14, and Theorem 5.18). Moreover,

$$f_0(z) = \int \frac{d\rho_F(x)}{1+xz}\,, \qquad f_1(z) = \int \frac{d\rho_K(x)}{1+xz}\,,$$

where ρ_F, ρ_K are the Friedrichs and Krein solutions of the moment problem. In particular, the moment problem is Stieltjes determinate if and only if $f_0 = f_1$.

There is a connection between $f^{[N+\ell-1,N]}(z)$ and the moment problems $\gamma^{(\ell)}$ and $\gamma^{(\ell-1)}$ (if $\ell < 0$, $\gamma^{(\ell)}$ and $\gamma^{(\ell+1)}$) given in Theorem 5.14 and Theorem 5.18. In particular, if $\ell > 0$ and $\gamma^{(\ell)}$ is Stieltjes determinate, then $f_{-1}(z) = f_0(z) = \cdots = f_{\ell+1}(z)$, and if $\ell < 0$ and $\gamma^{(\ell)}$ is Stieltjes determinate, then $f_1(z) = f_0(z) = \cdots = f_\ell(z) = f_{\ell-1}(z)$.

The situation for series of Hamburger is more complicated, but, in general, $f^{[N+\ell-1,N]}(z)$ converges for $z \in \mathbb{C}_+$ and $\ell = \pm 1, \pm 3, \dots$ (Theorem 5.31 and Theorem 5.32; see Theorem 5.31 for issues of existence of the Padé approximant).

There are connections between the Padé approximants and the polynomials P, Q, M, N as well as two finite matrix approximations $A_F^{[N]}$ and $A_K^{[N]}$ to the Jacobi matrix, A. $A_F^{[N]}$ is the upper right $N \times N$ piece of A. $A_K^{[N]}$ differs by adjusting the NN matrix element of $A_F^{[N]}$ so $\det(A_K^{[N]}) = 0$. Then

$$f^{[N-1,N]}(z) = \langle \delta_0, (1 + zA_F^{[N]})^{-1}\delta_0\rangle = -\frac{z^{N-1}Q_N(-\frac{1}{z})}{z^N P_N(-\frac{1}{z})}$$

$$f^{[N,N]}(z) = \langle \delta_0, (1 + zA_K^{[N+1]})^{-1}\delta_0\rangle = -\frac{z^{N}N_{N+1}(-\frac{1}{z})}{z^{N+1} M_{N+1}(-\frac{1}{z})}\,.$$

The connection to the continued fractions of Stieltjes is discussed after Theorem 5.28.

C6 Criteria for Determinacy.

Criteria for when a Hamburger problem is determinate can be found in Proposition 1.5, Theorem 3, Corollary 4.5, Proposition 5.13, Theorem A.6, and Theorem A.7.

Criteria for when a Stieltjes problem is determinate can be found in Proposition 1.5, Theorem 7, Corollary 4.5, Theorem 5.21, Corollary 5.24, Theorem A.4, and Theorem A.6. In particular, if one defines

$$\begin{aligned} c_{2j} &= \ell_j = -[a_{j-1} P_j(0) P_{j-1}(0)]^{-1} \\ c_{2j-1} &= m_j = |P_{j-1}(0)|^2 \end{aligned}$$

(the c's are coefficients of Stieltjes continued fractions; the m's and ℓ's are natural parameters in Krein's theory), then the Stieltjes problem is determinate if and only if (Theorem 5.21 and Proposition 5.23) $\sum_{j=0}^{\infty} c_j = \infty$.

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